UNIVERSITY OF MARYLAND
COMPUTER SCIENCE CENTER

COLLEGE PARK, MARYLAND

NASA RESEARCH GRANT NsG-398

Computer Oriented Research

in the

Space Related Sciences

Annual Status Report

March 1963 to March 1964

Dr. Werner C. Rheinboldt
Principal Investigator
Computer Science Center
University of Maryland

I. Summary of the Research Work

In March, 1963, the National Aeronautics and Space Administration awarded research grant NsG-398 to the Computer Science Center of the University of Maryland. This grant, entitled "Computer-Oriented Research in the Space Related Sciences", was given in support of a broad multi-disciplinary research program which is aimed at stimulating and broadening the effective use of large-scale computers in the University's extensive space research efforts, and at investigating new methods of computer applications in these fields.

In line with the above stated principal aims of the research program, the program itself concerns two interrelated areas of activity:

1) Research work on problems in the computer sciences to deepen our knowledge and understanding of the most effective use of computers in research. This includes investigative work on the design and implementation of programming and monitoring systems and their properties, research on special algorithmic languages and their compilers, as well as research in such areas of computer sciences as pictorial data processing and automatic pattern recognition, information storage and retrieval systems and computer-oriented mathematics.

2) Research work on the computer-oriented phases of a broad spectrum of space-related research projects in close cooperation with the individual investigators in the different academic disciplines. Such interdisciplinary research ranges from the analysis of methods for an effective computational approach to the problem, to the development of special techniques and appropriate programs aiding the investigators in all phases of their projects.

During the past year, intensive work has begun in both areas of the program. In the first problem area, emphasis was first placed upon the development of a versatile general purpose programming and monitoring system for the IBM-7090/1401, inasmuch as effective utilization of modern large computers in research is vitally dependent on the availability of such a versatile system. As outlined further in Chapter II, one primary goal has already been accomplished within this area and a flexible set of programming systems has been incorporated into one overall operational system which is proving itself to be extremely well adapted to the various demands of the research program. Other work concerned the development of special, general-purpose programming packages, notably for

multi-precision computations and for versatile input-output. Reports on these newly designed and developed systems have been written or are in preparation. In the coming year we plan to continue with the investigation and implementation of those general-and special-purpose systems which are particularly suited to the requirements of individual phases in the program - and with their incorporation into our total system.

A closely related research study has just been started which concerns non-sequential procedures and procedural languages as they occur in complex multi-computer and man-machine systems. The project is aimed at studying the logic of such procedures and at developing appropriate algorithmic languages and compilers capable of describing procedures without artificially specifying the order in which operations are to be carried out.

Whenever a research project involves a large amount and a great variety of complex computational work, the need for the development of special programming systems arises. The computer analysis of crystallographic structures in such a type of project, and with the support of the NASA grant, a first basic version of a flexible and effective crystallographic computing and programming system has now been completed. Even in its basic form, this system is already in use at various installations, such as the NASA Space Center at Huntsville, Alabama, and it is already beginning to achieve very gratifying and widespread recognition. The present system contains 15 program links, an additional 23 links are currently in various stages of planning and development. We are continuing this important work. Another and closely related project under way concerns the development of a similar programming system for the analysis of electrolyte measurements.

A few months ago work was started on a research project in the field of pattern recognition and pictorial data processing. This investigation involves the analysis of certain automatic pattern recognition problems by the computer synthesis of classes of patterns. More precisely, we wish to determine if, by the manipulation of higher order statistical dependencies (and other measures) within a picture, one can generate figures within a closed area which resemble certain meaningful shapes such as found in aerial photographs, cloudlike patterns, and similar patterns obtained, for example, in pictures taken from satellites and space vehicles.

Another project which has just been launched in the general area of computer science is concerned with investigating the special algorithmic structure of computer-based information storage and retrieval systems for handling literature in a narrow technical area, indexed in depth and with substantial detail and structure.

An integral part of this project is of course constituted by the investigation of the machine interphase for such an information system, and in this way the project is quite closely related to the more basic project concerning general non-sequential procedures, mentioned above.

So far, we have only mentioned some of the major computer-science oriented research work originating under the program. Additional, smaller projects of this type are described in Chapter II.

As a second area of activity under the program, we mentioned the close cooperative research work done on computer-oriented phases of a broad spectrum of space-related research projects. During the past year we have begun such cooperative work with a variety of investigators in different academic departments.

Some Specific Research Projects Within Area II:

Together with the Institute for Molecular Physics, a project is now under way in the general area of computer investigation of potential energy curves and wave functions for diatomic systems. In a first phase, a computation of vibration rotation matrix elements for diatomic molecules was completed. Intensive work is continuing at this time with the aim of 1) gaining detailed knowledge of the collisions between diatomic systems, 2) understanding the observed intensity distributions in diatomic band systems, and 3) interpreting the perturbations and predissociations in the spectra of diatomic molecules.

In the Department of Physics and Astronomy we have been cooperating with the newly established research work being done on radio astronomy. Computer programs have been developed for the reduction and analysis of long wavelength radio astronomical observations. We plan to continue this cooperation along the same lines and with the aim of developing a system of versatile and effective programs for the most efficient analysis of such radio astronomical observations.

Another area of cooperative work with the Department of Physics and Astronomy concerns the computational work in basic nuclear research. A number of relatively smaller projects are presently under way and will be described further below. Mention should be made, however, of a very interesting, new project in this field, which has opened up new areas of mathematical computer applications and involves computer investigations of the analytical properties of various functions in quantum field theory. Such an analysis of functions of several complex variables is undoubtedly

a completely novel use of computers and should prove to be highly important in a variety of fields.

In the field of Chemical Engineering we are doing cooperative work on the computer-oriented phases of several research projects, one of which concerns the study of liquid-liquid extraction and involves the computational analysis of fundamental mass transfer models for both continuous and dispersed phases in liquid extraction. Previous computational work of the investigators provided solutions for the general Hadamard model; this work is now to be extended to dropside and continuous models in order to include a wider range of flow conditions as well as continuous phase and interfacial resistance. Another project in Chemical Engineering involves a combined theoretical and experimental study on eddy transport coefficients and the analysis of the models on the computer.

In the Institute for Fluid Dynamics and Applied Mathematics a large-scale theoretical and experimental research study has been launched concerning rotating laboratory models which simulate the general circulation of the atmosphere. We are particularly interested in one very important computational part of this project, namely, the analysis and development of computational methods for the numerical prediction of circulations in such rotating models. This will necessarily lead to studies of various methods of numerical prediction employed in weather forecasting and of numerical approaches to general circulation models.

In connection with this cooperative work on the computer-oriented phases of various space-related projects, it should once again be noted that it is not our intention to support these individual projects directly. Any one of these projects involves a variety of other theoretical and experimental phases which in some instances have separate support; however, no support is available for the interdisciplinary research work on the associated computer science problems - or even for the planning of such interdisciplinary projects. When a computer is used as part of a research project, the high cost of the necessary equipment, problems of securing proper programming help, etc., often overshadow the entire computational effort and overstress the service nature of the computer work. At the same time, any serious research investigator knows that this service aspect is not the major consideration associated with the really effective application of computers. A highly significant contribution stems from the fact that the analysis undertaken to make possible the assistance of computers will often stimulate a type of feedback that casts new light on the research problem itself, thereby in turn serving to further the research effort.

PERSONNEL

Dr. W. C. Rheinboldt, Director of the Computer Science Center and Research Professor of Computer Science is the principal investigator of the entire program. Dr. Earl J. Schweppe, Dr. Richard Austing, and Dr. James Ortega, Research Assistant Professors of Computer Science, will work on various phases of the computer science research projects. In fact, Dr. Schweppe has already begun his earlier mentioned research on non-sequential procedures. Dr. Austing is taking the place of Dr. A. Sinkov who has left the University to go to Arizona State University. Dr. Austing's special interests are in computer-oriented mathematics. Dr. Ortega joined the Center in March 1964, his field of interest is numerical analysis and in particular questions of error analysis.

The programming systems work is under the direction of Mr. Alfred E. Beam, Senior Computer Systems Analyst of the Center, who works very closely with Mr. John P. Menard, Assistant Director of the Computer Science Center. The systems development group furthermore includes Mr. George E. Lindamood, Research Programmer at the Center. In addition, Mr. Robert Herbold, Computer Systems Analyst, joined the Center and this group in February 1964.

The research project on pictorial data processing and pattern recognition will be conducted by Dr. Nancy S. Anderson, Associate Professor of Psychology and Research Consultant of Computer Science, together with Dr. Azriel Rosenfeld, Research Associate Professor (P.T.) at the Computer Science Center. The programming part of this project is handled in part by Norman Simenson, Jr., Research Programmer at the Center.

The project on information structures and information storage and retrieval in depth is conducted by Dr. Howard Tompkins, Professor and Head of Electrical Engineering, together with Dr. Alan Marcovitz and Dr. James Pugsley, Assistant Professors of Electrical Engineering. We plan to appoint a Research Programmer for the programming work under this project as well as for Dr. Schweppe's closely related project on non-sequential procedures.

Mr. Charles K. Mesztenyi, Senior Research Programmer at the Computer Science Center, is directing the programming work connected with the research program. Under his guidance, Mr. Robert L. Clark, Research Programmer and Mr. Alexander Radichevich, Jr. Research Programmer, are working on special programming problems, such as the development of multi-purpose programs for use by different research projects. Mr. Mesztenyi is also continuing his work on rational approximations and plans to cooperate closely with the computer-oriented mathematical work under this program.

The following Graduate Research Assistants have been connected with the program during the Spring Semester of 1963: J. Connelly (Mathematics); G. Meyer (Mathematics); and S. Wax (Mathematics). C. Park (Chem. Engineering) and F. Karriker (Physics) worked with us full time furing the summer months. In the Fall semester of 1963/64 the following Graduate Research Assistants have been participating in the programs' activities: J. Connelly, F. Karriker,and C. Park. In the Spring Semester 1964, D. Wilson was added to this list.

Under the program, we plan to increase the number of graduate research assistantships from three to five, and three of these five assistantships should permit the student to continue with his program activities during the summer. The two additional students are to be assigned to the projects of Dr. Schweppe and Dr. Tompkins.

It should be noted here that three of the University's 30 NASA trainees are working in computer-oriented mathematics. They are: J. W. Snively, Jr., J. Maryak and P. Smith. These students have associated themselves closely with research projects under this program. J. Snively has just completed his Master's thesis with a computational project and Mr. Maryak is presently writing his Master's thesis on a similar program project.

In line with the multidisciplinary character of the entire research program, we are very fortunate to have the benefit of collaborating closely with the principal investigators of the various space-related research projects and their associates. The names of these University faculty members are listed under each of the specific projects in Chapter II.

FACILITIES

The computer-oriented work of the entire research program of course involves extensive large-scale computer use. This computer work is performed through the facilities of the Computer Science Center with its IBM-7090/1401 system, associated card handling equipment and large program library, while the services of the entire staff of the Center are employed.

In view of the nature and extent of the already existing, as well as the projected computer work, and in recognition of the importance of this work under the research program, the University decided to expand the computer system from an IBM-7090/1401 system to an IBM-7090/1460/1401 configuration. The change-over of the

IBM-7090 to the IBM-7094 and the delivery of the 8K IBM-1460 system is now scheduled for the Fall of 1964.

In order to accommodate the expanded computer system and to provide additional space for the continued growth of the Center's research activities, the University recently decided also to extend the basement and first floor of the present Computer Science Center building (possibly by the end of 1964) by the addition of approximately 9,000 square feet.

II. Details of the Research Work

The following chapter describes in more detail the individual projects which were undertaken under the research program. The presentation is intended to provide a picture of each project as a whole, that is, a description of the scientific background and purpose of the project whenever possible, together with an account of the actual computer-oriented phase of the project - which is of course the main concern of our program here. A summary of the most significant projects is given in Chapter I. For the sake of convenience, we here provide a list of all titles in the order of presentation in this Chapter:

(1) Programming Systems

(2) Research in Non-Sequential Procedures

(3) Research in Pattern Recognition and Pictorial Data Processing

(4) Information Storage and Retrieval in Depth

(5) A Computing System for Crystallographic Structure Determination

(6) Development of a Computing System for the Analysis of Electrolytes

(7) Mathematical Logic and Machine-Proving of Theorems

(8) Potential Engergy Curves and Wave Functions for Diatomic Systems

(9) Analytical Properties in Quantum Field Theory

(10) Scintillation Counter Spectrum Analysis

(11) Long Wavelength Radio Astronomy Research

(12) Mass Transfer Between a Dispersed Liquid and a Liquid Continuum

(13) Turbulent Transport Coefficients

(14) Geophysical Fluid Dynamics

(15) Abstracts of Selected Additional Computer-Oriented Research Projects

(16) Projects Presently Completed or Nearing Completion

(17) Abstracts of Selected Additional Projects Started since December 1963

A list of all Technical Reports describing some of our accomplishments under the program is given in Appendix I. Appendix II gives a detailed breakdown of the computer time used under the entire program.

(1) Programming Systems

Principal Investigators: Alfred E. Beam, Senior Computer Systems Analyst
John P. Menard, Assistant Director, Computer Science Center

In cooperation with: Gerald M. Berns, Systems Engineer, IBM-Corporation

As was pointed out earlier, the effective utilization of modern complex large-scale computers depends crucially on the availability of versatile programming and monitoring systems. Especially for a multidisciplinary research program such as ours, the proper selection, adaptation and diversification of highly flexible programming systems is of the utmost importance. Accordingly, we concentrated heavily on the development and modification of such systems.

Our work in this area can be categorized as follows:

(a) Incorporation of a versatile set of programming systems into one overall operational system.

(b) Development of new general purpose programming systems and packages and their incorporation into the overall system.

(c) Investigative work on ALGOL and ALGOL compilers.

(d) Development of special purpose programming systems for individual research projects with complex computing requirements.

Our work in the first category can best be described with the aid of figures 1 and 2 at the end of this section. Figure 1 shows all the individual systems which have been integrated into our principal operational system, which in turn is especially suited to the configuration of our equipment and the special needs of our research program. Figure 2 shows all our other operational systems available to the researcher using our facilities. In the development of the principal system (figure 1) we began with the basic IBM monitor (IBSYS), adapted it to our needs, and incorporated a variety of special systems such as the list-processing systems LISP and IPL-V and the tabular language OMNITAB of the National Bureau of Standards. We are presently working on the incorporation of the Michigan Algorithm Decoder (MAD), and plan to continue this type of developmental work in accordance with the special requirements of the entire research program. For example, the need for simulation languages (e.g. SIMSCRIPT of GPSS) has already arisen. Other work in this area will of course concern the adaptation of our entire programming systems to the new configuration of our computer system now on order.

In the second category, we have concerned ourselves with the development of multiple-precision packages and versatile input-output systems. A special multiple precision system (MPP) for performing computations requiring very high accuracy on a large range of data has been developed by A. Beam and is described in our Technical Report TR-63-3, October 1963. For ease of operation and to give greater accessibility to MPP, the so-called PRECISE system, patterned after OMNITAB, has been worked out by A. Beam. Both systems are operational under our main system (see figure 1).

Another line of investigation has now resulted in a system called MOIST (Macro Output Input SysTem). As indicated by its name, the purpose of MOIST is to provide an extremely flexible and simple means for programming input and output for the IBM-7090/94. MOIST has been written using IBMAP and operates under our main system. (Technical Report TR-64-5).

We plan to intensify this work on new general purpose systems during the coming months. In particular, the research projects on non-sequential procedures (see II (2)) and on information structures (see II (4)), call for the design and implementation of several such systems.

With the increasing importance of problem-oriented, general algorithmic languages, it became necessary to devote a certain amount of our attention to ALGOL and ALGOL compilers. We have made the SHARE-ALGOL compiler available for our research program, and a short time ago we undertook a study of the Stanford BALGOL compiler. Furthermore, the Computer Science Center has joined the ALCOR group and we are now actively cooperating with the University of Illinois and the Technical University of Munich, Germany, in the field testing of the ALCOR-ALGOL-7090/94 compiler.

As mentioned earlier, whenever a research project involves a large amount and a great variety of complex computational work, the need for the development of special programming systems arises. As described in Section (5) of this Chapter, we are cooperating with Dr. J. Stewart in his work on the X-ray 63 crystallographic computing system and we began work with Dr. Atkinson (see II (6)) on the design of a programming system for the analysis of electrolytic measurements. This type of work on special purpose programming systems and their incorporation into the main operational systems is expected to constitute an increasingly expanding part of the work of our programming systems group during the coming year.

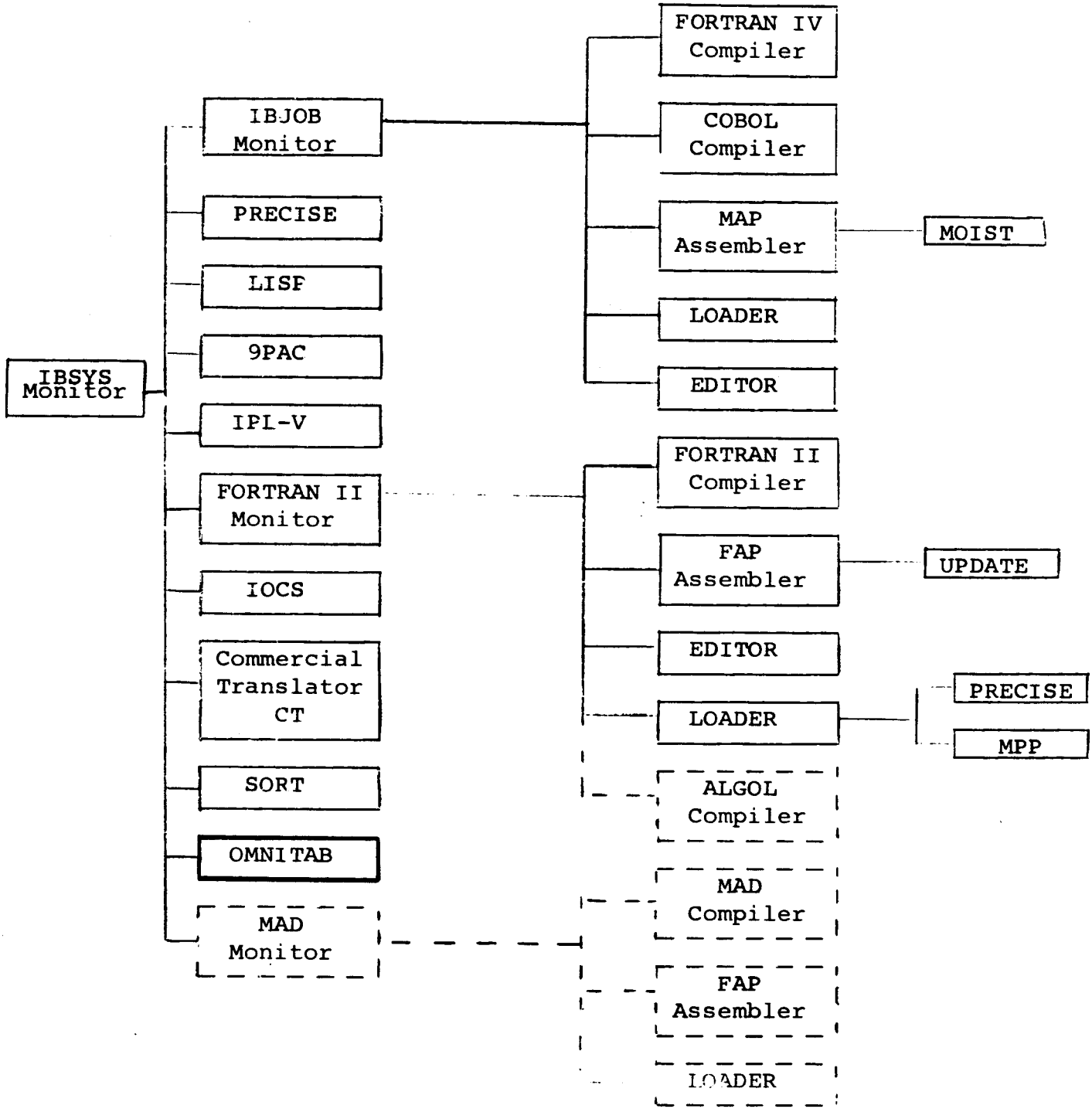


Fig. 1

Primary Operating system at the Computer Science Center. Dashed lines indicate those systems presently being made operational under the IBSYS Monitor.

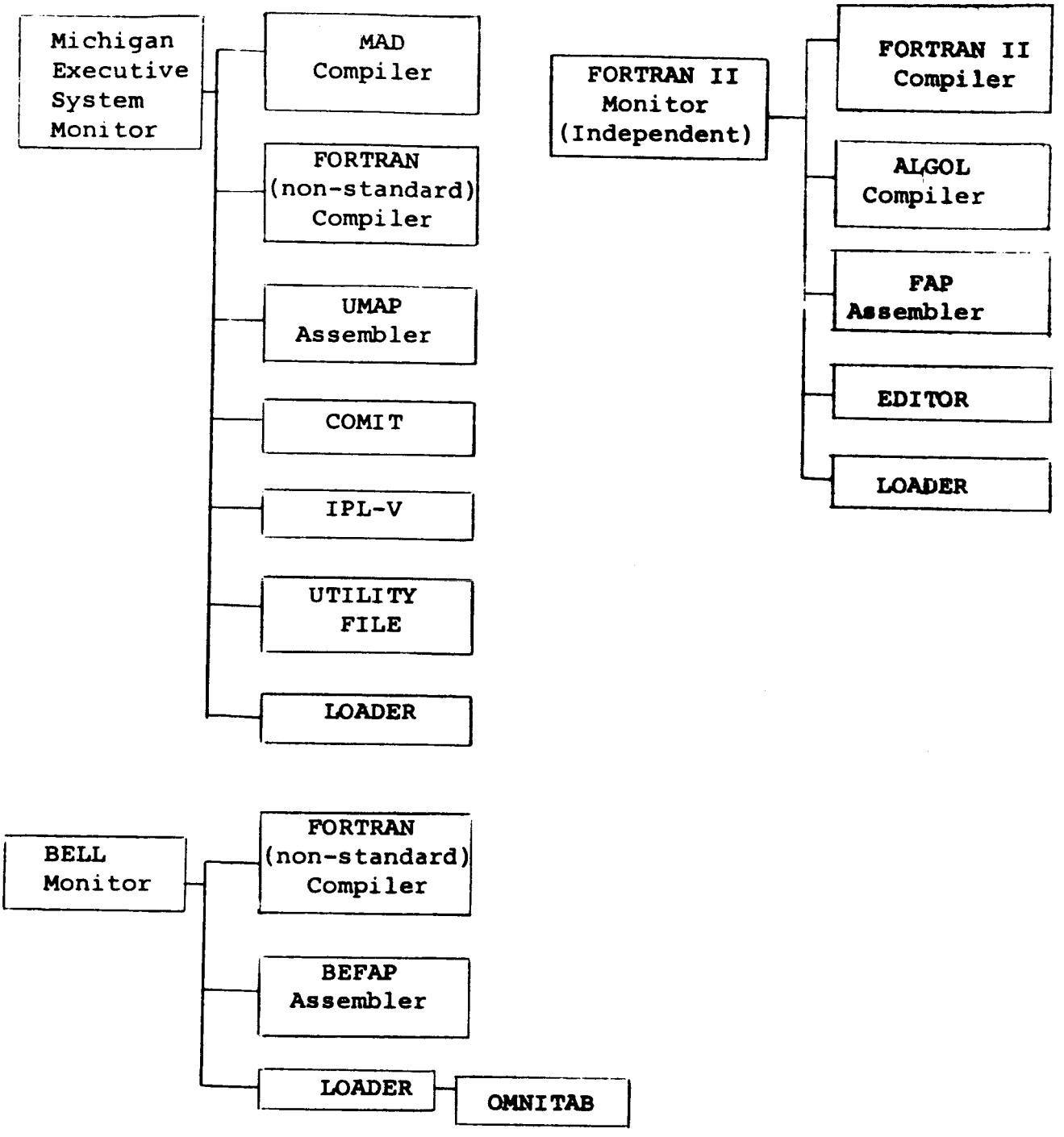


Fig. 2

Other systems that are operational and presently available upon request at the Computer Science Center.

(2) Research in Non-Sequential Procedures

Principal Investigator: Dr. Earl J. Schweppe, Research Assistant Professor, Computer Science Center

In August 1963 Dr. Schweppe joined the faculty of the Computer Science Center and from that time he has assumed a very active role in this research program. His interests are in the study of procedural languages and their associated programming systems; in particular, in the study of non-sequential procedures as they occur in complex multi-computer, man-machine systems, and, in line with this, he has recently begun a research study of such non-sequential procedural languages.

Most of the developments which have taken place to date in computer science have been based on stating programs and carrying out events in a sequential manner. Thus even in the more sophisticated algorithmic languages, as well as in macro, assembly and machine languages, the order in which the statements are written is sequential, and so is the order in which they are carried out--except, of course, for specific decision points where the linear flow of control may be changed. The early machines were themselves highly sequential in design and so it was natural that the development of languages should follow this pattern. In a strictly sequential system, however, no two events may occur at the same time and thus the individual parts of the computer are used only a small percentage of the time.

Recent years have seen many efforts to increase the efficiency with which equipment is used. Independent data channels, look-ahead, and memory overlapping features have been used for some time. More recently, the development of highly parallel machines, following the work of Holland, as well as of multiple computer systems, have moved fairly far in this direction. As in the case of the sequential machines, the development of programming languages to take advantage of these new features is lagging behind the development of the machinery, although there have been a number of efforts in recent years to use sequential machines in a non-sequential manner. For example, we find various time and memory sharing systems in use or in development, especially in real time applications.

As every programmer and machine designer knows, among the many steps in most procedures, the order of execution is often not critical. It would frequently be possible to do things in parallel and, in fact, the machine designer often does not take advantage of such situations. The programmer on the other hand is very limited in using these situations and must state one sequence

or another in his program. The facilities which are available to overlap operations are for the most part highly machine dependent and usually available only in a language close to that of the machine. Procedures which have been described sequentially contain many subtle dependencies which are not easy to analyze. For example, it is quite difficult to take advantage of the possibilities for overlapping operations when the language used specifies many artificial, sequential dependencies.

When processes of a larger scale are studied, the need for a non-sequential means of expression and operation are even more evident. This may be seen in the development of the simulation languages and management aids. Thus PERT, SIMSCRIPT, GENERAL PURPOSE SYSTEM SIMULATOR and other similar systems contain many non-sequential features which indicate the trend of the future.

The research underway is initially a broad, theoretical, as well as practical study of the logic of procedures themselves. As this study progresses, one of the primary concerns is that of developing notation and language capable of describing procedures without artificially specifying the order in which the operations are to be carried out. In this work, it is necessary to consider both the language used to program non-sequential procedures, as well as the language in which the user asks for such a procedure to be carried out. As such languages are developed, it is necessary constantly to consider the logic and form of both machinery and executive control which might be able to execute and supervise procedures described in such a way. Although the possibility to use these techniques on sequential machines of conventional design has already been demonstrated, it is expected that the results of this study will have significant long term effects on the logical organization of hardware as well as software.

One system which employs some of the first results of this study is under construction by the Ames Laboratory at Iowa State University, Ames, Iowa. This system is to be used in real time asynchronous control and data logging in experiments conducted around a new atomic reactor.

(3) Research in Pattern Recognition and Pictorial Data Processing

Principal Investigators: Dr. Nancy S. Anderson, Associate Professor of Psychology and Research Consultant, Computer Science Center

Dr. Azriel Rosenfeld, Research Associate Professor (P.T.), Computer Science Center

Mr. Norman Simenson, Junior Research Programmer, Computer Science Center

Since the Summer of 1963, Dr. Anderson has been actively participating in the research activities of the Computer Science Center. Dr. Anderson's interests are in the area of pattern recognition and pictorial data processing. Her efforts to establish a research program at the Center in this highly important field were greatly augmented when in October 1963 Dr. Rosenfeld joined the Center as part-time Research Associate Professor.

Jointly, Dr. Anderson and Dr. Rosenfeld are now undertaking a research project in the field of pattern recognition and pictorial data processing. In particular, the research is aimed at extending the techniques used thus far for recognition of classes of patterns similar to those with space oriented applications such as those pictures taken from satellites and space vehicles. The over-all importance of this research area in relation to space research in general need of course not be stressed here again.

a) Pattern Analysis by Synthesis: The processing of pictorial data by general purpose digital computers presents many challenging problems to the computer programmer and the applications engineer. The human observer's ability to perceive and recognize pictures in "real time" appears to depend heavily on certain special-purpose processing mechanisms which are far from completely understood.

Many problems in the area of pictorial data processing and pattern recognition relate to the fact that pictures and patterns are not completely arbitrary, but rather represent a familiar reality (photographs) or a formalized symbolism (printed matter). In a general pictorial pattern recognition situation, a set of measurements is made on a given picture or pattern, and the results of such measurements are compared with the corresponding measurements for a class of reference pictures. (The class may be implicitly or explicitly given.) Based on the results of these comparisons, a recognition decision is made which "assigns" the given picture to an appropriate subclass. The measurements used to provide the "recognition data" may at one extreme involve the

pictures in toto ("template matching") or, at another extreme, the measurement may involve sampling processes of properties of the picture such as spatial frequency analysis and correlation integration.

The distinguishing characteristics of a picture or pattern may be found in a specific portion of it rather than the picture as a whole. (A "figure" in the picture can be distinguished from the rest of the picture by properties of luminance distribution, higher order statistical distributions of the occurrence of white, black or gray portions, etc.) To measure such recognition data, figures must first be extracted from the picture. In many character recognition situations, there is a high degree of figure standardization in terms of luminance (black on white), orientation, and size. In many scientific photo interpretation situations there may be little or no standardization, and patterns are perceived as a result of the human observer's ability to perform highly complex perceptual processes.

A number of recent automatic photo interpretation studies such as described by Holmes, et al (1962), have devoted considerable effort to the figure extraction problem. Furthermore, since Attneave (1954), as well as others, has shown the important information of certain classes of patterns to be found at the contour, several studies such as Julesz (1962) have investigated the methods by which contours or figures in a picture may be generated. Many of these investigations have indicated that certain measures of redundancy of areas within the picture (or measures obtained from cross correlation techniques between a mask shaped like the figure and the picture, Holmes et al (1962)) do result in the identification (or extraction) of figures.

The investigations now underway involve the analysis of certain automatic pattern recognition problems such as described above by the synthesis of classes of patterns. The computer is used to generate classes of patterns by randomly filling cells of matrices or areas enclosed by curved lines with black, white or gray. These patterns will then be changed by mathematical or statistical techniques to investigate further the usefulness of certain measures to describe figures within pictures. That is, we wish to determine if by manipulation of higher order statistical dependencies (and other measures) within a picture, one can generate figures within a closed area which resemble certain meaningful shapes such as found in aerial photographs or cloudlike patterns. For example, the changing of higher order probability distributions in a random field of black and white squares in a matrix can introduce an identifiable figure area of the picture as different. (Julesz (1962)) The

parameters of these higher order probability distributions could thus be used in an automatic recognition system to identify edges of figures, textural changes in certain areas, etc. The present investigators plan to extend these techniques, as described above, to non-rectangular patterns (areas enclosed by curved lines) and to generate two or more discriminably different figures within the enclosed area. The computer as a high speed data processor is particularly suited for the business of generating and modifying by mathematical and statistical computations classes of patterns which contain certain kinds of figures. Experimental studies will be conducted to evaluate these techniques for generating figures within synthetic patterns by performing scaling and recognition studies with human subjects.

At present a computer program has been written to generate classes of patterns with black and white squares. These patterns of black and white squares are generated in a matrix of maximum size 50 x 120 cells, (see Figure 1). All cells of the matrix are white or black with an average probability of one-half. The patterns are generated as follows. Each line is statistically independent of all other lines and the probability of any line beginning with a black or white run is 1/2. Thereafter, black and white runs alternate. The independent variable is the probability of the length of the runs which may vary from one to four cells.

The probability distributions of white and black run lengths are independently controlled, except that, to maintain uniform density of black and white ($p(B) = p(W) = 1/2$ as noted above), the means of the black and white run length distributions must be equal. The lines are generated from the "midpoint" out, so that all truncation of runs occurs at the outer boundaries; but the "midpoint" can be arbitrarily placed at any point from the extreme left to the extreme right of the matrix.

The right half of the matrix can differ from the left half by manipulation of the higher order statistical dependencies among the cells. These changes are made by varying the parameter of the probability distributions of the black and white run lengths (under external program control). The choice of parameters for the first set of over one hundred patterns has been made, and sets of patterns will be generated this spring. A series of experiments will be conducted to determine what values of the parameters are discriminably different, and on what stimulus dimensions these judgments are based.

In addition to generating synthetic patterns of black and white cells in matrices, plans are nearing completion for the outline of computer programs to be used in generating sets of patterns using alphanumeric and special characters. Studies by Neisser (1961) have indicated what rules are used by people to search for a change in patterns made up of columns of letters and numbers. Experiments conducted with figures within a pattern generated by changing the shape of the character will add further valuable information about people's ability to recognize discrepancies in texture in visual search tasks.

Essentially, the approach described above is one of analysis by synthesis. The investigators want to extend the previous studies of techniques for detecting edges and textures by using these techniques to generate classes of patterns with recognizable figures within them. The particular techniques to be used will be those suggested Julesz (1962), Holmes, et al (1962), Giuliano (1961), Hu (1962), Rosenfeld (1962), Horowitz (1961) and others. In addition, certain studies of human pattern recognition, Anderson and Leonard (1958), indicate that redundancy per se does not alter human pattern recognition in a consistent manner. Certain types of redundancies aid in the human's ability to recognize contour, and other types of redundancy hinder recognition performance. Investigations of the different methods of generating certain figures within pictures and subsequent psychophysical studies using human observers may add insight into the complex role of different kinds of redundancy in influencing visual pattern recognition by human observers. For example, in generating texture changes and contour boundaries in the patterns described above, certain of the higher order probability distributions may enhance edge detection by observers for patterns of different levels of detail, (or alternatively under optimum viewing conditions with respect to visual angle distortion, etc.)

b) Analysis of Connected Regions of a Given Brightness on an Image: A relatively elementary but non-trivial image processing problem is that of separating out connected components in an image. As examples one can cite: The "countries" defined by the borders on a line map; the connected pieces of cloud on a cloud cover image. A program for assigning a different label to each such component in a given image, and computing the areas of the components, has been written. A refined program which also computes "dimensions" for the components is currently in progress. By dimensions we mean here the lengths of the sides of the rectangle with largest shorter side which can be inscribed in each component.

c) Simulation of a Concept for Frequency Encoding an Image: If the brightness at each point of an image is modulated at a different frequency, and the resultant total brightness is measured over a sufficient time period, the image can be reconstructed by Fourier analysis. Certain approximations to the required modulation pattern are relatively easy to produce. A signal-to-noise analysis for one such approximation has been programmed; the results indicated that the approximation is inadequate. Other approximations are currently under consideration, but no programming has been done for them as yet.

d) Synthesis of Stimuli for Studying "Visual Texture": Mr. J. Slattery, Jr. a graduate student at the University currently has an assignment involving the synthesis of a set of "pseudo one-dimensional" visual stimuli (random-down, constrained across), using overstrike printout techniques, similar to the ones described above in study (a). As those more general patterns of study (a), these one-dimensional stimuli will also be used in an exploratory psychological study. One-dimensional visual texture parameters which are expressible in terms of constraints on the distributions of "white" and "black" run lengths, are of particular interest in this project.

e) Simulation of a Novel Tool for the Quantitative Study of Shape: A method for shape analysis in which the contour of the given shape "propagates" parallel to itself, and in which self-intersections of the propagating contour play a crucial role, has been proposed in an unpublished paper by Mr. H. Blum of the Air Force Cambridge Research Laboratory. This method has important implications for the quantitative definition of basic shape parameters ("piecedness", elongation, etc.) as well as for the psychology of form perception. A general approach to its computer simulation has been sketched out, but time has not yet permitted programming it.

REFERENCES

Anderson, N. S. and Leonard, J. A. The recognition, naming and reconstruction of visual figures as a function of contour redundancy, J. Exp. Psychol., 1958, 56, 262-270.

Attneave, F. Some informational aspects of visual patterns, Psychol. Rev., 1954, 61, 183-192.

Giuliano, V. E. Automatic pattern recognition by a Gestalt method, Information and Control, December, 1961.

Holmes, W. S. et al, Design of photo interpretation automation, Cornell Aeronautical Lab. Proc., FJCC, December, 1962.

Horowitz, L. P. Autocorrelation pattern recognition, Proc. IRE, January, 1961.

Hu, M. K. Visual pattern recognition by moment invariants, IRE Trans. on Info. Theory, February, 1962.

Julesz, B. Visual pattern discrimination, IRE Trans. on Info. Theory, February, 1962.

Neisser, U. Time analysis of logical processes in man, Proc. West. Joint Computer Conf., 1961, 579-585.

Rosenfeld, A. Automatic recognition techniques applicable to high-information pictorial inputs, IRE Inter. Conv. Conv. Record, March, 1962.

Figure 1: Pattern matrix generated by random runs of overstruck characters

(4) Information Storage and Retrieval in Depth

Principal Investigators: Dr. Howard E. Tompkins, Prof. and Head
Dr. Alan B. Marcovitz, Assistant Prof.
Dr. James H. Pugsley, Assistant Prof.
Department of Electrical Engineering

in cooperation with: Dr. Earl J. Schweppe, Research Assistant Prof., Computer Science Center

Work has begun toward the development of a computer-based information storage and retrieval system well adapted to the storing of the literature of fairly narrow technical areas, indexed in substantial detail.

Background for the Research in Information Storage and Retrieval:

Computer-based systems for the storage and retrieval of technical information have, so far, made use of relatively unstructured sets of descriptors or keywords (1). A good comparison of this approach against the use of a hierarchical classification scheme has been given by Doyle (2), who details several reasons for introducing some structure among the descriptors.

Doyle (2), Gurk and Minker (3), and Sams (4) all emphasize the importance of good communication between the computer and the user of the system, if any structure inherent in the document description scheme is to be used effectively.

Cost and technological limitations have so far mitigated against the practical use of highly structured information stores indexed depth. However, there have been several research efforts in this direction, largely aimed at the programming and file structure problem. Sams (4) and Colilla and Sams (5) have expressed what they consider to be fundamental requirements for such systems, including "the need to identify index terms as belonging to a class...which permits a set of subsuming relations between elements in the class...(and) among the classes themselves." They hoped to be able to limit the needed structure of index terms to tree form.

It seems probable that more complex structural forms will be needed. Barnes (6) applies graph theory to part of the problem, confining himself to the description of the"cognitive content" of a topic statement defining the document being indexed. The resulting structures for single articles are lattices, and these must co-exist by the thousands.

Not only will computer programs to cope with such complex linguistic structures be large, but they must be flexible, to adapt to changing needs and increasing insight (7).

Outline of Research Plan

The plan of the research that has begun is outlined below, then discussed in more detail.

PHASE 1

A) Selection of areas of research as subject areas in which to practice the storing and retrieving of research results. A preliminary choice of two areas is
   1) Mechanized Information Storage and Retrieval
   2) Theory of Sequential Systems

B) Development of a suitable structure for indexing in depth in the selected areas.

C) Hand simulating a sample of the developing experimental indexing structure.

D) Selection of the most suitable available programming language for 7090 simulation of a larger sample of the experimental indexing structure, and execution of the 7090 simulation.

PHASE 2

A) Evaluation of the results of Phase 1 with particular regard to the needed improvements in
   1) indexing structure
   2) programming
   3) man-machine communication
   4) machine configuration

B) Acquisition or development of needed man-machine communication equipment, and machine configuration.

C) Extension and improvement of the programs and indexing structure to the point where a realistic comparison of structured indexing in depth versus the then available versions of coordinate and keyword indexing is possible.

Phases 1 and 2 as sketched will take at least three years. Phases 1A and 1B now in progress.

Discussion of Research Plan

Mechanized Information Storage and Retrieval has been tentatively selected as one of the literature areas to be studied because of the obvious value of the stored (and retrieved) information to the conduct of the research. The Theory of Sequential Systems has been selected because it is an area to which both of the Assistant Professors who are working on this research have devoted research effort in the past (8,9).

We believe firmly that progress on information storage and retrieval systems depends on having a balanced program of theoretical and practical effort, involving substantial competence in the subject area being indexed. These considerations have guided our choice of subject areas.

The proposed indexing structure consists of a set of interconnected information lattices or "subspaces" (e.g., spaces for author, location, topic, item, document, concept, etc.). Points in these subspaces interact in two ways, through characteristic or intrinsic relations between the points that are independent of specific information items, and through linkages caused directly by specific information items. The structure of storage for the points, linkages, and intrinsic relations in topic space is still in a formative stage, but is based on list processing techniques, and conforms to the following principles:

1) It is possible to locate all references to a particular point or to a particular information item, in whatever subspaces they may be, so that corrections, changes, and deletions may be made completely, accurately, and efficiently.

2) It is possible to progress transitively through the structure, an any appropriate subspaces, with a minimum of blind searching, while following logical or associative paths from one point to another, either under automatic program control or semi-automatic control by the user.

3) It is possible to use widely varying levels of detail in establishing descriptions, so that brief mention of less consequential items is possible, and is not incosistent with very detailed consideration of an important information item.

4) It is possible to include in the structure auxiliary information such as citations, in such a form as best utilizes the clues they contain as to topic (10).

Preliminary consideration indicates that these conditions can be met, hopefully with a structure of manageable size and complexity.

An immediate research goal is the completion of enough details of the structure to permit an adequate hand simulation of its use, followed by a machine simulation as soon as is practicable. An extensive programming effort is required to get suitable macros established to cope with our manipulative needs. The existing special languages for information retrieval and hueristic programming, for example COMIT and IPL-V, do not appear to be completely suitable for our needs. A firm decision at this time seems unwise; a decision should be made in the next few months.

Throughout phase 1 we shall be accumulating and indexing suitable technical information, storing it for retrieval, and making such improvements in index structure and programming as are needed.

One additional feature of the projected information storage system concerns the way the structure will be used.

A major problem with any information system involving detailed indexing is the problem of human inconsistency. Not only will two humans index the same information differently, but the same human, at different times, will index a single item differently. These facts impose two requirements on an information system, flexibility and metaconsistency.

Flexibility implies the facility to accept and keep track of changes upon changes, without an unusable snarl resulting.

Metaconsistency implies the existence of efficient procedures for calling inconsistencies to the attention of the user, in effective ways. For example, when an item is indexed, the system should respond by relating that item to others that have similar indexing--preferably only to the "closest" ones, in a suitable sense. The system should then present to the indexer the pattern of other items having similar indexing, and the structure of previously used index terms closest to those prescribed for the current item, and should ask if any modification of the indexing is desired.

In other words, a trial retrieval of the new item and others closest to it should be immediately available to the indexer, to help him fit the new item in as appropriately as possible.

In the special case of re-indexing a previously indexed item, which should be permitted, the system should accept the new indexing, compare it in toto with the prior indexing, and comment helpfully by displaying the differences. If two indexers are involved, who persist in disagreeing, the system should be able to preserve that fact.

It is expected that the lack of a suitable man-machine interface console will interfere with the most effective use of the system. Also the lack of an appropriate mass storage will hurt. As soon as is feasible, these problems should be considered, and solutions mapped out.

The carrying out of these solutions is the first order of business for phase 2 of the effort, along with a full evaluation of the index structure and programming.

Finally, a realistic comparison, on economic and utilitarian grounds, of unstructured retrieval versus the achieved system, is desired.

REFERENCES

Nonconventional Technical Information Systems in Current Use, No. 3, pp. 100-124, National Science Foundation, October 1962.

Doyle, Lauren B. (SDC, Santa Monica, California), "Semantic road maps for literature searchers," J.A.C.M., vol. 8, pp. 553-578, October 1961.

Gurk, H. M., and Minker, Jack (RCA, Princeton, N. J.), "The design and simulation of an information processing system," J.A.C.M., vol. 8, pp. 260-270, April 1961.

Sams, B. H. (RCA, Bethesda, Md.), "On the solution of an information retrieval problem," Proc. 1963 SJCC (AFIPS Conf. Proc., vol. 23), pp. 289-297; Spartan Books, Baltimore, Maryland, 1963.

Colilla, R. A., and Sams, B. H. (RCA, Princeton, N. J.), "Information structures for processing and retrieving," Commun. A.C.M., vol. 5, pp. 11-16, January 1962.

Barnes, Robt. F. (Itek Labs, Lexington, Mass.), "Language problems posed by heavily structured data," Commun. A.C.M., vol. 5, pp. 28-34, January 1962.

Sams, B. H. (RCA, Princeton, N. J.), "Dynamic storage allocation for an information retrieval system," Commun. A.C.M. vol. 4, pp. 431-435, October 1961.

Marcovitz, A.B. (U. of Maryland, College Park, Md.), Lin-Time-Varying Discrete Systems, Ph.D. Thesis in Electrical Engineering, Columbia University, June 1963.

Pugsley, J. H. (U. of Maryland, College Park, Md.), Linear Sequential Machines Whose Logic Elements Contain Delay, Ph.D. Thesis in Electrical Engineering, University of Illinois, June 1963.

Salton, Gerard (Harvard U., Cambridge, Mass.), "Associative document retrieval techniques using bibliographic information," J.A.C.M., vol. 10, pp. 449-457, October 1963.

(5) A Computing System for Crystallographic Structure Determination

Principal Investigator: Dr. James M. Stewart, Assistant Prof. of Chemistry and Research Consultant, Computer Science Center.

From the start of our multidisciplinary research program Dr. J. Stewart has participated in this effort continuing to pursue his work on the development of a flexible and effective crystallographic computing and programming system.

The problem of accurately determining the atomic parameters in crystals from X-ray or neutron diffraction data of solid crystalline material is of the greatest importance for scientific research today. When the data are obtained by diffraction rather than refraction methods, the use of high-speed computers is of crucial importance to the practicality of the method for investigating the structure of the many interesting compounds.

In the beginning of programming for the solution of crystal structures, it was common practice to write isolated programs for each application. However, as diffraction techniques improved and data gathering became more automated, it became clear that the programming methods would also have to improve and become more automatic.

Dr. Stewart's work is concerned with the development of methods and computer programs for the crystallographic structure determination, and with the integration of these computer programs into a much needed crystallographic computing system.

At this time a first goal of this work has been accomplished, and the basic core of the crystallographic computing system has been completed. A list of programs at the end of this section gives an indication of the intended scope of the entire system for the IBM-7090/7094. At present there are 15 completed "links" in the system (indicated by asterisks). Dr. Stewart is now working on the design and implementation of the remaining 23 programs as well as on their incorporation into the system.

The partly completed system has already received widespread recognition and has been distributed for use at various

universities and U. S. Government installations, including the NASA-Space Center at Huntsville, Ala.

Summary of the Research Project: The set of IBM-7090 programs which constitute the "X-ray System" are designed to perform all the computations necessary for the accurate determination of the atomic parameters in crystals from X-ray or neutron diffraction data of solid crystalline material. A few main programs constitute the "backbone" of the system while the remainder performs all accessory computations that aid in the interpretation of the results and prepare the results in the form of readable output.

The programs are interrelated to constitute a self-contained computing system for X-ray crystallography which will run independently of, or in conjunction with, any existing IBM-709/7090/7094 monitor systems.

The following is a description of three of the principle programs, their function, inter-relation, and some of their main features.

The data reduction program serves to prepare a binary tape upon which are stored the crystal cell dimensions, space group symmetry operations, and reflection intensity values (reduced to relative structure amplitudes). This initial program calculates $\sin^2 \frac{\theta}{\lambda^2}$ for each reflection and by means of a 4 point interpolation gets the scattering amplitudes for each atomic species directly from literature values. Every effort is made to protect later programs, which may be used many times, from calculating quantities which the data reduction program can store on the binary "reflection" tape. Thus cell constants, maximum values of h, k, ℓ, (the Miller indices), the interpolated values of the scattering factors, and the symmetry information for each reflection are all stored in a form useful for structure factor, Fourier transform, least-squares, and differential synthesis calculations.

The space group symmetry is read into the data reduction program in the form of a set of general equivalent coordinates expressed in the same form as they appear in the International tables for X-ray crystallography. These key-punched letters are then transformed into a set of rotation matrices and translation vectors. These matrices may in turn be used by

subsequent programs to generate the necessary symmetry. Settings outside those listed in the International tables may be used. Two of the programs mentioned above, namely the structure factors program, and differential synthesis program use these matrices. They are also required for bond length and angles computation, Fourier refinement and other calculations done by the system. If the vector of the Miller indices H = (h,k,ℓ) is operated upon by the rotational part of the symmetry operation a new set of Miller indices results which is the set for a symmetrically equivalent reflection. The phase of this reflection in relation to the unique reflection supplied at data reduction time is given by the "fringe function."

The "fringe function" may be catalogued by the dot product of the unique reflection and the translation vector of the symmetry operation modulo one. Since the only allowable translations in the crystallographic space groups are halfs, thirds, quarters and sixths, the list of possible resulting "fringe functions" is very short (i.e. 0, 1/6, 1/4, 1/3, 1/2, 2/3, 3/4, 5/6). Therefore it is very practicable to generate equivalent reflections for the Fourier and least-squares program by means of this stored information.

Thus, even though the structure factor, Fourier, least-squares, and other programs are based upon the calculations for Triclinic cells much of the work of generation is done at data reduction time, thereby easing the calculation load of the later more often used programs but at the same time providing generality with respect to space-groups and settings treated.

The structure factor program calculates

$$F_{C(h,k,\ell)} = \sum_{j=1}^{N} f_j \exp(-T_j) \exp(-2\pi i(hx_j + ky_j + \ell z_j))$$

from a supplied "unique" set of atomic coordinates and the binary tape prepared by the data reduction program. The temperature parameters may be overall or individual, isotropic or anisotropic temperature factors. The program handles atoms in special positions without the need for patching or special intervention. The "triclinic" set of atoms is generated from the "unique" set supplied by means of the rotation matrices and translation vectors stored at data reduction time. As each atom is generated it is checked to assure that it does

not lie on a special position. If it does, suitable information is printed out and the atom scaled appropriately.

The program will also calculate Templeton dispersion corrections, rescale factors and $R = \frac{\Sigma \Delta F}{\Sigma F_o}$ for the observed reflections.

The Fourier program calculates

$$\rho(x,y,z) = \frac{1}{V} \sum_{h,k,l} F_{o(h,k,l)} \exp(2\pi i(hx + ky + lz))$$

for any desired grid interval, from any origin, for a large number of reflections, for all space groups in any setting. The fringe function codes stored at data reduction time generate the set of equivalent F amplitudes from the unique observed ones and the calculation is then carried out as if the cell were triclinic. There are limits on the fineness of the grids and the maximum number of reflections for the second and third sum directions. Because of the method of summation the maps printed out may be made in grid intervals that result in undistorted maps for orthogonal sections.

The summations are carried out for as many levels as possible in one pass along the reflection tape. The program makes the necessary calculations to decide how many passes will be required by the available storage. The user therefore supplies only the desired number of divisions along each axial direction, the number of points desired in each direction, the interval in divisions between points, the point of beginning, the layout of the resulting map (e.g. x across, y down the page) the desired spacing between lines, and the coefficients to be used (e.g. ΔF, F_o, F_c etc.).

All the details of space group setting and map symmetry are taken care of by the program itself.

The course of the computation which may involve any number of the links in the system is controlled by the sequence of cards in the input data. These control functions are exercised by a special subroutine called "CALLER" through which all input passes. Input data cards are identified by punches in the first six card columns, usually a mnemonic of the card function. A data deck consists of the following kinds of cards:

(a) Operational cards (which are acceptable at any time) perform immediate operations such as assigning tapes, printing remarks and instructions and supplying a title.

(b) A calling card serves to call the specified program link and initiate the program.
(c) Data cards to be used under control of the program and to supply, for example, parameters, intensity data, and control information.
(d) An end card indicating the end of the data deck.

A sequence of interdependent calculations may be performed by stacking up an appropriate set of data decks, for example, "parameter loading" followed by a "Fourier synthesis," or several cycles of "automatic refinement." This set of data decks is identified by a preceding special card, the *-data card. Another independent sequence of calculation may be initiated by following the first sequence by another *-data card and one or more data decks --at continuum. Execution terminates and control is returned to the calling monitor when a "FINISH" card or an END-OF-FILE is read on the monitor input tape.

The list of program links at the end of the section serves to illustrate the present and intended scope of this crystallographic computing system for the IBM-709/7090/7094. The asterisks indicate the programs currently included in the working systems tape.

At present there are "checked out" 15 links of the X-ray system. While these links consitute a core of the calculations of crystal structure determinations there remain a number of other necessary, useful and time-saving links to be added. Twenty-three of these links are at present in various stages of check-out, conversion from other computer languages, coding and planning stages. They fall into several broad categories:

(1) Aid in data gathering (e.g., GE-XRD 5, Eulerian Craddle settings, correlation of intensity data from various sources, e.g., films, counters, etc.)

(2) Aid in interpretation of solved structures (e.g., bond length and angles, projection of a molecule on an arbitrary plane in space, thermal parameter geometry).

(3) Phase determination (e.g. Karle-Hauptman computations, Patterson superposition).

(4) Systems links (e.g., list generation for data publication, program library maintenance, tape copying).

The major responsibility for the "X-ray 63" programming system lies with J. M. Stewart (University of Maryland) and Darrell High (University of California at San Diego). The programming as a whole has been the result of group effort by many people. J. Stewart is currently preparing a report giving a complete description of the system and the methods used.

X-ray Crystallography System--List of Library Programs:

This list is the table of library programs in the "X-ray 63" programming system. An asterisk refers to the programs currently included in the working system tape.

*	LOADER	Beginning program, tape generation
*	FC	Parameter loader and statistical calculation of structure factors
*	DIFSYN	Differential synthesis
	DFSYNA	Modified differential synthesis
	LSQFM	Full-Matrix least squares
*	ORFLS	Busing-Martin-Levy full-matrix least squares
*	FOUREF	Fourier refinement (shifts atoms to Fourier peak)
*	SHLPAT	Shell Patterson
	BONDLA	Bond length and angles
	PROJCT	Projection of a molecule on a plane
*	LSQPL	Least squares, plane and line.
	SUPTAP	Preparation of superposition binary tape
	SUPERA/SUPERB/SUPERC	Patterson superposition programs A, B and C
	SUPROT	Rotation program to fit model to Patterson
*	DELSIG	Plot of delta-F versus F-observed for sigma for data reduction
	PHASE	Calculation of Karle-Hauptman phases
*	DATRDN	Data reduction
	DATCOR	Data correlation for films
*	DATFIX	Calculation of scaled unitary structure factors
*	MODIFY	Search and modify reflection tape
	WEIGHT	Prepare weights for least squares
*	ESORT	Sort for Karle-Hauptman phase determination
	LISTFC	Final structure factor listing
*	FOURR	Fourier synthesis

*	CRYSET	Donnay-Takeda crystal transformations
*	RPLANE	Calculate R over a projection for moved molecule
	RLIST	Calculate R for special classes of reflection
	PARAM	Least-squares refinement of lattice parameters
	TFINFO	Calculates temperature factor statistics
	GESET	Generation of reflection and crystal set for GE XRD-5
	REFPAK	Interconverts reflection tape and binary deck
	REFSOR	Reflection sorting from tape
	TAPCOP	General tape copying routine
	PATCON	Patterson convolution program
*	BYEBYE	Convert system reflection tape to non-system formats
	NRLA/NRLB	Spare entry A or B, respectively for experimental purposes
*	ERLINK	Execution error diagnostics program

(6) Development of a Computing System for the Analysis of Electrolytes

Principal Investigator: Dr. G. Atkinson,
Assistant Professor of Chemistry

Dr. G. Atkinson is directing a research group involved in an extensive program of measurements in electrolyte solutions. At the present time these measurements concern low field conductance, high field conductance, transference numbers, EMF of cells, Wien effect dispersion, dielectric constant, and the absorption and velocity of ultrasonic waves in solution.

The analysis of these measurements depends critically on the use of modern large-scale computers. Most electrolyte measurements have a solid theoretical foundation; this theory must be used in the data analysis when meaningful results are to be obtained. Yet the various theories have varying degrees of validity and even one particular theory often differs in validity for different electrolyte systems. It is therefore necessary to couple the reduction of measurement data to a sophisticated comparison and analysis of the theory in order to gain adequate certainty about the entire data analysis.

This in turn requires the development of a large variety of methods and programs for the computer analysis. Moreover, as in the case of the analysis of crystallographic data, these computer programs have to be integrated into a complete computing system for electrolyte analysis, if the computer work is to be effective. The development of such an electrolyte analysis system is urgently needed and is of critical importance to the practicality of the research programs concerned with the many interesting electrolyte solutions.

Dr. Atkinson and his students are now undertaking the design and development of such a computing system for the analysis of electrolyte measurements. As in the case of the "X-ray 63" system of Dr. Stewart (see the previous section), the system will consist of an interconnected set of program links which perform the various types of analysis; it will aid in the interpretation of the results and prepare those results in the form of readable output.

The entire project will undoubtedly continue for several years. We are now supporting the design of this computing system under our present NASA grant. The continuation of this support

over the next year will be very critical for the entire project since the principal lay-out of the core of the system will be undertaken during this year, which in turn will substantiate the fundamental correctness of this system's approach.

Rather than present brief descriptions of the problem in each of the above measurements, we will here present a more detailed description of one of the measurement analysis problems in particular.

Ultrasonic Absorption: In recent years, use of so-called "relaxation techniques" for the investigation of solution processes has led to new insights into solution behavior. One of the most versatile relaxation methods is the measurement of ultrasonic absorption as a function of frequency.

The theoretical background of this technique has been described in a recent article by Tamm and Eigen (1). In general one can say that in electrolyte solutions any equilibrium process involving a ΔV can give rise to sound absorption in the solution in excess of that in the solvent. A plot of excess absorption per wavelength versus frequency will show a maximum for each such equilibrium process. The positions of such maxima are directly related to the rates of the equilibrium, and the amplitude of the maxima are related to the ΔV for the process and the actual equilibrium constant.

In some recent work (2) Dr. Atkinson and his group examined $MnSO_4$ in water and mixed solvents. Aqueous $MnSO_4$ solutions exhibit relaxation maxima at 3Mc, 35Mc, and 220Mc. It can be shown that all three peaks are due to the ion assocation process

$$Mn^{+2}\ (aq) + SO_4^{-2}\ (aq) \rightleftharpoons MnSO_4\ (aq)$$

The three peaks mean that this process takes place in three distinct steps which can be written in the following way.

$$\underset{(1)}{Mn^{+2}\ (soln)} + \underset{(1)}{SO_4^{-2}\ (soln)} \underset{k_{21}}{\overset{k_{12}}{\rightleftharpoons}} \underset{(2)}{Mn^{+2}\ (S\text{-}S)\ SO_4^{-2}} \qquad (I)$$

$$\Big\downarrow k_{23} \qquad \Big\uparrow k_{32} \qquad (II)$$

$$\underset{(4)}{MnSO_4} \underset{k_{43}}{\overset{k_{34}}{\rightleftharpoons}} \underset{(3)}{Mn^{+2}\ (S)\ SO_4} \qquad (III)$$

Where S = solvent molecule; and all molecules of solvation are ignored except for those between the ions. For such a coupled reaction scheme, the relaxation times are given by:

$$\frac{1}{\tau_I} = k_{21} + k'_{12}$$

$$\frac{1}{\tau_{II}} = k_{32} + \left(\frac{k'_{12}}{k'_{12} + k_{21}}\right) k_{23} = k_{32} + k'_{23}$$

$$\frac{1}{\tau_{III}} = k_{43} + \left(\frac{k'_{23}}{k'_{23} + k_{32}}\right) k_{34} = k_{43} + k'_{34}$$

where $k'_{12} = k_{12}^{\circ} \alpha c f_{\pm}^{2} \left(2 + \frac{\partial \ln f_{\pm}^{2}}{\partial \ln \alpha}\right)_c$

α = degree of dissociation
$f_{\pm}$ = mean activity coefficient
C = stroichiometric concentration
$\frac{1}{\tau_i} = 2\pi\nu_i$
ν_i = frequency of peak maximum in CPS

Because of the intricate relationships between the rate constants in the above scheme Dr. Atkinson developed a slightly different approach to the data analysis. From Eigen's work it is quite apparent that τ_I (corresponding to the 220 Mc peak) is due to the diffusion controlled approach of the two completely solvated ions. Therefore it was assumed that the equilibrium constant for this step is given by the Bjerrum model taking the Bjerrum distance as the sum of the ion radii plus two solvent molecule diameters.

$$K_{12} = \frac{c_1^2 f_{\pm}^2}{c_2} = \frac{K_{21}}{k_{12}} = \text{Bjerrum } K$$

$$K_{23} = \frac{c_2}{c_3} = \frac{k_{32}}{k_{23}}$$

$$K_{34} = \frac{c_3}{c_4} = \frac{k_{43}}{k_{34}}$$

and

$$K_{\Sigma} = \frac{c_1^2 \, f_{\pm}^2}{c_2 + c_3 + c_4}$$

Under the assumption that K_{12} is known from the Bjerrum model, all six rate constants can be calculated from the variation of the $\nu_M'^s$ with concentration. The results for aqueous solution show that the new approach to the data interpretation is extremely satisfactory.

This work has been extended to dioxane-water and methanol-water systems and to temperature dependence. Papers are now in preparation utilizing the rate constant, ΔV and E_A parameters obtained by computer analysis. The work is being extended to C_oSO_4 and to M_gSO_4 (an important seawater constituent).

A computer program has been developed which evaluates all the terms involving the $f_{\pm}$ and its variations, finds the frequencies of maximum absorption and evaluates the rates and equilibrium constants. Now the work is extended to the computer analysis of the actual absorption values in terms of for each step and the equilibrium constants. In all these cases the analysis is simplified by the good separation of the relaxation frequencies. As the frequencies come close together a more advanced method of computation has to be employed using the transformation matrix approach to analyze the experimental frequencies in terms of the rate constants.

This brief description of one of the data reduction problems gives some idea of the scope of the extensive computing system envisaged. Some of the other measurements involve the processing of much more data with even more complicated theories. The programs developed so far, and which are now under development, are expected to have value for all chemists and biologists

interested in electrolytes, long before these programs have even formed a self-contained computing system.

(7) Mathematical Logic and Machine-Proving of Theorems

Principal Investigator: Dr. S. Kuroda,
Professor of Mathematics

Since the start of our research program, we have cooperated closely with Professor Kuroda in his research project on computational methods in algebraic number theory. This investigation aims at clarifying structures of the ideal class group of cyclotomic fields Q_m (ζ_m) generated by a primitive root of unity ζ_m where m is a positive integer related to the rational primes of

$$q = (p^r - 1) / (p^d - 1) \quad (p \text{ rational prime})$$

A related problem involves the determination of the decomposition law of rational primes in various algebraic number fields.

As a first phase of this research it becomes necessary to compute prime number tables which are more extensive than those generated up to now. This in turn has lead already to very interesting computational problems. During the past half year a set of computer programs has been developed to calculate a table of all prime numbers less than 4.29 billion in a form suitable for further computations. All programs have been developed with the hope of achieving utmost efficiency, proper generality, and usefulness in further number-theoretic and logical computations. It is particularly noteworthy that the programs are extremely fast. For example, to compute a table of prime numbers in an interval of about 1.8 million numbers takes only between 39 seconds to 140 seconds, depending on the location of the interval in the total range from 0 to 4.2 billion. A report [2], submitted to NASA, describes these programs in detail.

We supported this research project under our NASA-grant until Professor Kuroda received a special NSF grant for the continuation of this work in the Fall of 1963.

Parallel with this research project, Professor Kuroda returned recently to some of his previous work in mathematical logic on the problem of machine-proving of theorems.

Mathematical logic can be regarded as one of the theoretical foundations of computer science. The problem of theorem-

proving by machines, in particular, is one of the basic problems in abstract computer science and in the theory of algorithms.

Professor Kuroda's research plan is based on his earlier studies of the logical structure of mathematics ([3] to [14]) using a new logical system which he formulated in [3] as a simplification and generalization of the system of Gentzen. The new system is, in fact, mechanically so simple that it merits testing as a tool for proving mathematical theorems by computer. This kind of work is being done by several investigators but it has for the most part been limited to proving formulas of pure logic. Professor Kuroda is now undertaking the planning of a computer program which is adequate for providing storage for concepts belonging to various areas of mathematics. Some of Professor Kuroda's ideas of such machine proofs were presented in [14] and were incorporated in 1959/60 in a program written under his direction by T. Takasu for the M1 computer of the Electrical Communications Laboratory of the University of Tokyo, Japan. Although the M1 computer has a capacity of only 512 40-bit words, this program produced machine proofs of a class of theorems such as

$$a \subseteq b \Rightarrow \sigma\restriction a \subseteq \sigma\restriction b$$

where $\sigma\restriction a$ is the restriction of the mapping σ to a (see [14]).

References

H. Cohn, O. Taussky, Number Theory in, Survey of Numerical Analysis, edited by J. Todd, McGraw-Hill, 1962.

S. Kuroda, J. Maryak, On Sieves and Primes Technical Report 63-2, Oct. 1963, Computer Science Center, University of Maryland.

S. Kuroda, An Investigation on the Logical Structure of Mathematics (I) A. Logical System, Abh. University of Hamburg, 22, 1958, 242-266.

S. Kuroda, (II) Transformation of Proof, Abh. University of Hamburg, 23, 1959, 201-227.

S. Kuroda, (III) Fundamental Deductions, Nagoya Math. J., 13, 1958, 123-133.

S. Kuroda, (IV) Compendium for Deductions, Nogoya Math. J., 13, 1958, 134.

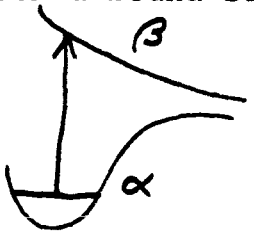
S. Kuroda, (V) Contradictions of Russel's Type, J. Syrub. Logic, 23, 1958, 393-407

S. Kuroda, (VI) Consistent V-System, Nagoya Math. J., 14, 1958, 109-127
S. Kuroda, (VII) Set Theoretical Contradictions, Nagoya Math J., 15, 1959, 109
S Kuroda, (VII) Consistency of the Natural Number Theory T_1 (N), Nagoya Math. J., 14, 1958, 129-158
S. Kuroda, (IX) Deductions in the Natural Number Theory T_1 (N), Osaka Math. J., 11, 1959, 7-42
S. Kuroda, (X) Concepts and Sets, Osaka Math. J., 11, 1959, 213-248
S. Kuroda, (XII) The Principle of Extensionality and of Choice, Proc. Japan Academy, 34, 1958, 400-403.
S. Kuroda, (XIII) A Method of Programming of Proofs in Mathematics for Electonic Computing Machines, Nagoya Math. J., 16, 1960, 195-203

(8) Potential Energy Curves and Wave Functions for Diatomic Systems

Principal Investigators: Dr. J. Vanderslice, Professor
Dr. S. Weissman, Assistant Professor
Dr. W. Benesch, Assistant Professor
Institute for Molecular Physics

One of the aims of the research project is the interpretation of the observed absorption coefficients for diatomic systems to obtain information on repulsive curves. Normally, the continuous absorption of radiation is due to a transition from a bound state of the system to one or more repulsive states. Under certain assumptions, the absorption coefficient α_ν is proportional to the overlap of the wave function of the states involved in the transition, i.e.



$$\alpha_\nu \sim \int \psi^{\alpha}_{\nu,r}\, \psi^{\beta}_{\nu,r}\, dr$$

Some work has been done on the evaluation of this matrix element assuming certain empirical forms for the potential curves and hence for the wave functions. Stueckelberg (1), for example, assumed a harmonic oscillator bound state and a linear function for the repulsive state. Bayliss, Rice, and Gibson (2) assumed a Kraetzer potential for the bound state and an inverse square dependence on the distance for the repulsive state. Under the direction of the investigators of this project, S. K. Luke recently succeeded in evaluating the integral for a harmonic oscillator - exponential repulsion combination (3).

None of the above combinations are completely realistic, of course, since the various empirical functions often do not correspond exactly to the correct potential curves for a given system although the exponential function is generally considered to be the most realistic. A Morse curve-exponential repulsion combination would perhaps be the most satisfactory combination of empirical functions to use. On the other hand, previous work of the investigators (4), (5) has shown that the bound curve can usually be obtained very accurately from the band spectra of diatomic molecules. Once the curve is known accurately, the wave function can be computed numerically by computer methods (6). This latter wave function together with the wave function for an exponential repulsion for the upper state is perhaps the best combination to use in interpreting the absorption coefficient data for most cases. A comparison of the observed and computed adsorption coefficients should then serve to determine the parameters in the exponential function.

Thus, since the potential curves and the radial part of the wave functions can now be determined from experimental data on both bound and repulsive states, a number of problems can be considered. Franck-Condon factors can be calculated and by comparison with experimental intensity distributions, the variation in the electronic transition moment for various types of transitions can be estimated. This leads to additional information on the electronic wave function. At the moment, we are considering the Franck-Condon factors and the transition moments for the different forbidden transitions in N_2 using the recent results of Tilford, Wilkinson and Vanderslice on these systems.

A closely related problem is that of the interpretation of observed perturbations and predissociations in the spectra of diatomic molecules. Mulliken (8), in an excellent paper, has discussed qualitatively the effects of different types of curve crossing on the observed predissociations in diatomic molecules. He indicates that the predissociation depends sensitively on the overlap integral:

$$\int \psi^{A}_{v,r} \, \psi^{B}_{v,r} \, dr$$

for the two states involved. To discuss this quantitatively, one has to have quite accurate wave functions which can be obtained by computer methods once reliable potential curves are known. Since, as indicated, the problem of bound states is well in hand, then the determination of repulsive curves accurately from absorption coefficient data will enable us to handle all the different cases that will arise. There are a number of cases for which experimental data on perturbations and predissociations are known and for which accurate potential curves are available -- CN being the most promising one -- which can be used to test the calculations.

W. Benesch concerned himself with the computation of the vibrational matrix elements for dipole transitions of a rotating diatomic molecule. He developed several IBM-7090 programs for finding the matrix elements for individual vibration rotation lines.

The first program generated matrix elements based on the Morse oscillator wave function and the following dipole moment function

$$M = M_o + M_1(r-r_e) + M_2(r-r_e)^2 + M_3(r-r_e)^3.$$

The values obtained with this program have been very helpful in the interpretation of data resulting from hydrogen iodide intensity measurements. The measured and computed matrix elements

are in good agreement in both the fundamental and the overton bands although the development of certain trends at the highest values of the rotational quantum number, J, indicated that the centrifuqal stretching might have been treated more rigorously.

In an effort to improve the J-dependence of the results, the next program developed was based on perturbed harmonic oscillator wave functions suggested by Herman and Wallis and on the dipole moment function (1). As a result of the inclusion of an additional term in the expansion of the centrifugal stretching term, the J-dependence of the results was, indeed, improved, so that these computations consitute the best theoretical representations of the fundamental line intensities of hydrogen iodide and hydrogen bromide.

Since the potential function upon which the Herman and Wallis wave function is based is quite unrealistic, the computations which are most successful in the fundamental band are not readily extended to the overtone band. Accordingly, it was considered worthwhile at this point to turn to a direct numerical integration of the radial Schroedinger equation appropriate to this problem. Methods were developed for computing wavefunctions by direct integration based first on a Morse potential function and most recently on an RKR potential function as calculated according to the scheme of Weissman et al.[9] The latter procedure greatly broadens the generality of the program, and initial comparisons have indicated that it will lead to considerable improvement in the theoretical interpretation of the measured dipole matrix elements. Current efforts are being directed to the application of the method to all diatomic molecules for which intensity data exists.

REFERENCES

(1) E. C. G. Stueckelberg, Phys. Rev. 42, 518(1932).
(2) G. E. Gibson, O. K. Rice, and N. S. Bayliss, Phys. Rev. 44, 193(1933).
(3) S. K. Luke, Master's Thesis (to be published).
(4) J. T. Vanderslice, E. A. Mason, W. G. Maisch and E. R. Lippincott, J. Mol. Spectroscopy 3, 17(1959); 5, 83(1960).
(5) W. R. Jarmain, Can. J. Phys. 38, 217(1960).
(6) James W. Cooley, "Some Computational Methods for the Study of Diatomic Molecules" AEC R&D Report, N.Y.U., May 1, 1961.
(7) J. T. Vanderslice, S. Weissman, E. A. Mason, and R. J. Fallon, Phys. of Fluids 5, 155(1962).
(8) R. S. Mulliken, J. Chem. Phys. 33, 247(1960).
(9) S. Weissman, J. T. Vanderslice and R. Battino, J. Chem. Phys. 39, 2226(1963).

(9) Analytical Properties in Quantum Field Theory

Principal Investigator: Dr. J. Toll, Professor and Chairman
Dept. of Physics and Astronomy

Under Dr. Toll's direction a group of theoretical physicists in the Department of Physics and Astronomy has been investigating the analytical properties of various functions in quantum field theory that are of particular interest in the theory of elementary particles. This has led to a very novel use of high-speed computers and represents a type of computation which, we expect, will be much more widely used in the future. The elementary particle interactions are usually described in terms of diagrams such as the one in Fig. 1. In this figure the momenta of the various ingoing and outgoing particles are represented for 4-dimensional vectors. From the axioms of quantum field theory it can be shown that any such general interaction involving N particles is a boundary value of an analytical function of these vector components. It is trivial to show, in most cases, that these functions are analytic in certain tube domains in which the imaginary parts of the difference vectors of these momenta are in specified light cones. However, the points of physical interest are not in this primitive domain of analyticity, but are in the boundary of this domain.

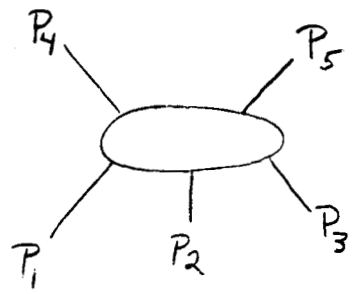


Fig. 1

Again using the axioms of quantum field theory it is possible to show that the scattering functions depend on the vector components only through the Lorentz invariants and the only analytic invariants are all functions of the invariants of the inner products $Z_{ij} = p_i p_j$. One is interested in determining what is the actual domain of analyticity in these invariants p_i p_j. The larger the domain of analyticity, the greater are the restrictions implied by this problem on the physical theories. Studies of these analyticities have led to proofs of dispersion relations which permit one to determine coupling constants, to relate high energy and low energy scattering, etc.

The primitive domain in the Z_{ij} can be extended by noting that many different scattering functions are equal on certain boundaries so that a single function is analytic in the union of

certain domains. A major problem in recent years in quantum field theory has been to find the final holomorphy envelopes for these various scattering functions under various physical assumptions, and the program is still only in the beginning stages.

The work at the University of Maryland, as at many other centers, proceeds in two different ways. First, various model theories are developed which can be solved only to a given order by expansion in terms of particles of a coupling constant. Such "perturbation theory" calculations have been made by many workers. In addition, a few workers have been trying to determine analyticity domains by use of the basic axioms of the quantum field theory without determining the particular structure. Kallen and Wightman[1] determined the analyticity domain of the 3-point function under general axioms when there are no "mass restrictions". This domain is extended when one introduces known information about the lower limit on the masses of possible intermediate states. This "3-point domain with mass restrictions" has been studied by W. S. Brown[2] of Princeton University and by Kallen and Toll[3]. The 3-point function, or vertex function, is the special case when there are only three momentum vectors involved, and in this case there are three independent invariants. Thus, the vertex function is an analytic function of three complex variables. The "domain without mass restrictions" of Kallen and Wightman[1] was bounded by seven analytic hyperfaces. Brown[2] has shown that several of these surfaces are penetrated when mass restrictions are introduced, and he solved the question of the new boundary in a particular case.

Kallen and Toll[3] showed that the most general vertex function could be given a convenient integral representation, three-fourths of which was closely related to certain perturbation theory diagrams (which have been called the Mercedes diagrams). Thus, the general axiomatic problem has been partly reduced to a study of certain perturbation theory diagrams. Because the computations of the singularity manifolds are so difficult, the electronic computers have been found to be very useful. It is not feasible to try to compute the whole surface in the space of six dimensions - instead, the computer is used to gain insight into particular situations, after which the results suggested by the computer are then proved, whenever possible, by other methods and then generalized.

A code has been developed and used to determine the singularity manifolds of the double triangle diagram of Fig. 2.

This diagram involves two closed loops and therefore the corresponding analytical function can be represented by an integral over two internal momenta with five denominators corresponding to the five internal lines.

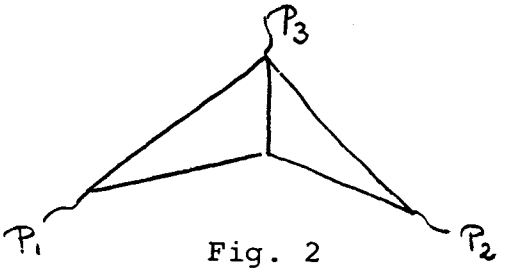


Fig. 2

Singularities develop when the integral contours are pinched between the singularities of several different denominators. The most complicated possible single manifold comes from a "total pinch", in which all the denominators vanish. On the basis of the numerical calculations it was first conjectured and later proved that the "total pinch" for this diagram is irrelevant in the principal Riemann sheet, and this result was later proved by analytic methods.

The computer is now being applied to the study of the Mercedes diagram (Fig. 3). In this case the determination of the position of the "total pinch" involves the solution of an 8th degree polynomial equation in some cases and a 12th degree polynomial equation in other cases. Programs have been developed at both Lund and Maryland to solve these equations and to calculate the trajectories of the "total pinch" manifold as an internal mass is varied. This work is still in progress, but it is hoped that it will give an insight into the total role of the Mercedes program's place in determining the final boundaries of the 3-point domain with mass restrictions.

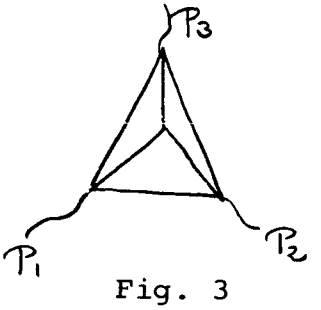


Fig. 3

Subsidiary programs have also been developed to calculate the envelope of the singularity domain for the simple triangle domain (Fig. 4) with mass restrictions, since this provides a convenient starting point for the more complicated equations mentioned above.

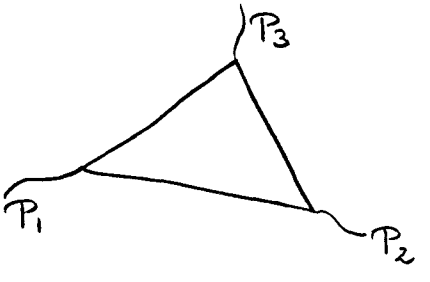


Fig. 4

In addition to the study of the 3-point domain, some work has also been done on the 4-point domain. In his Ph.D.

dissertation at the University of Maryland, A.C.T. Wu[4] computed the simplest 4-point diagram (Fig. 5) in terms of 128 dilogarithms and studied the resulting domain in six complex variables. Kallen and Toll[5] proved that the primitive domain for the 4-point function is already much more complicated than that of the 3-point function in that the boundary is not an analytic hypersurface. However, Jost[6] has recently shown that the primitive 4-point domain can be parameterized conveniently by the DANAD formula. Wu[7] has recently shown that a perturbation theory diagram can be described by a simple change in the DANAD formula so that one now has two cases of the DANAD formula between which the final boundary must lie. Wu's result again demonstrates the usefulness of perturbation theory diagrams for suggesting the final singularity domain. Thus, there is good reason to hope the 4-point domain will be discovered by studying examples from perturbation theory, using high speed computers.

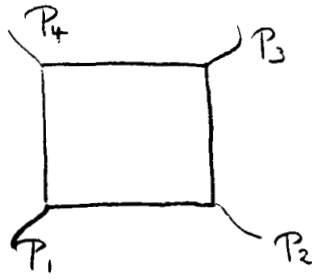


Fig. 5

While the fundamental problem mathematically is to determine the analyticity domain in all invariants, a simple problem of particular physical interest is to study the case when the p_i^2 are given by the squares of known real masses. In this way, the number of complex variables is greatly reduced and the 4-point function is, for example, reduced to the elastic scattering amplitude which is a function of two complex variables. Within a more restricted domain one can ask "What is the most general domain for this function of two complex variables?" The well-known Mandelstam representation is based on a conjecture that this function $A(s,t)$ is analytic, except for three cuts along the real axes of s, t, or u, where $u = m^2 - s - t$. Perturbation diagrams have been discovered which violate this conjecture, but it is still not known whether, under certain mass restrictions, the conjecture might still be satisfied in cases of physical interest. The investigators have been attempting to investigate this in various ways. Professor Y. Kim has been trying to devise examples of perturbation theory diagrams which would violate the Mandelstam representation even in the simplest case of equal masses, but so far his program is incomplete. Kim and Toll[8] have also been trying to construct models of scattering amplitudes, consistent with Lorentz variants, with crossing symmetry and unitarity. To do this, they have gone over to new variables which are crossing symmetric and they have used our IBM 7090 to

solve the 6th degree equations necessary to determine the image of the Mandelstam domain in these new variants. They expect to use the computer in their future attempts to generate models by the iterated application of the unitarity condition.

In the future the group also hopes to apply the computer to the direct construction of holomorphy envelopes in several complex variables. However, the procedures for this work are still under development.

References:

G. Kallen and A. S. Wightman, Mat. Fys. Skr. Dan. Vid. Selsk. 1, No. 6 (1958).

W. S. Brown, Jnl. Math. Phys. 3, 221 (1962) and Ph.D. Dissertation, Princeton University.

G. Kallen and J. S. Toll, Helv. Phys. Acta 33, 753 (1960).

A.C.T. Wu, Mat. Fys. Medd. Dan. Vid. Selsk. 33, No. 3 (1961).

J. S. Toll, Proc. Naples Conf. (1959) in Lectures on Field Theory and Many Body Problem, Academic Press (1961), pp 147.

R. Jost, Proc. Naples Conf. (1959) in Lectures on Field Theory and Many Body Problem, Academic Press (1961),pp. 142.

A.C.T. Wu, "Perturbation Analyticity and Axiomatic Analyticity: I. Connection of Landau Equations with Jost DANAD Manifold", Harrison Randall Laboratory of Physics, University of Michigan (to be published).

J. S. Toll, Bull. Am. Phys. Soc. 8, 393 (1963).

(10) Scintillation Counter Spectrum Analysis

Principal Investigator: Dr. Robert Detenbeck, Assistant Prof.
Dept. of Physics and Astronomy

Nuclear scintillation counters are used to measure the energy distributions of particles emitted in nuclear reactions. The distribution in voltage of the pulses obtained from the counter is related to the energy distribution of the particles. In order to obtain the particles' energy distribution, the experimenter must "unfold" the instrumental response to each monoenergetic component. The problem is further complicated by noise in the measurement, arising from statistical counting uncertainties.

In the past, the unfolding process has involved inversion of a large matrix (say 20 x 20 or 40 x 40) for each measurement. This has required the use of a large computer (say a 7090), which cannot be easily accessible to the experimenter while he is running. It is often very important for the experimenter to have at least a rough idea of his results immediately. During the summer of 1963 the author studied the problem of using a large computer before the experiment to prepare tables that the experimenter can apply to complete a preliminary data analysis with only a desk calculator. Such tables prepared by the large computer can be used over and over on a group of similar experiments; the large calculation (perhaps 15 minutes on an IBM 7090) need be performed only once for the whole group.

The procedure for unfolding spectra is mathematically equivalent to a least-squares fit to a number of discrete energy components. However, the method of calculation avoids the matrix inversion commonly used in this area of data analysis. Briefly, the fitting procedure is this. We are given a set of data points, y_i, which consist of the numbers of counts in pulse-height channels i = 1, ..., N. Typically, N = 250. For each of M standard (say 40) gamma-ray or neutron energy components, there is a standard count-distribution, $x_{\lambda i}$. We wish to write the best approximation to y_i of the form

$$\sum_{\lambda=1}^{M} A_\lambda x_{\lambda i}$$

that is, to minimize the quantity

$$\sum_{i=1}^{N} \left(y_i - \sum_{\lambda=1}^{M} A_\lambda x_{\lambda i} \right)^2 .$$

It must be assumed, of course, that the x_λ are linearly independent. If from the M linearly independent vectors x_λ an orthonormal set w_λ is constructed by

the transformation

$$(1) \quad w_\lambda = \sum_{\mu=1}^{M} \Gamma_{\lambda\mu} x_\mu \;, \qquad \lambda = 1, \ldots, M \;,$$

then by applying the adjoint we can construct

$$(2) \quad V_\lambda = \sum_{\mu=1}^{M} \Gamma_{\mu\lambda} w_\mu$$

The least-squares solution to the problem, for any on A_λ is then given by

$$(3) \quad A_\lambda = \sum_{i=1}^{N} V_{\lambda i} Y_i$$

Thus, from a computer-calculated table of V_λ the experimenter can extract from his data y any coefficient A_λ by the simple summation given in (3). The rms uncertainty in A_λ from counting statistics is given by an equally simple expression:

$$(4) \quad \Delta A_\lambda = \left[\sum_{i=1}^{N} (V_{\lambda i})^2 Y_i \right]^{1/2}$$

It is possible to modify the method in a trivial way to allow for a weighted least-square fit. However, the weights will not generally be known before the experiment is performed, and equal weights are more practical.

The primary advantage of this method of calculation has been the insight it affords into the fitting procedure. For example the relationships between energy resolution (spacing of components) and the amplification of counting fluctuations by the fitting process are being studied with satisfying results. Also, an additional degree of freedom in fitting has become apparent which reduces the effects of inaccurate spectrometer energy calibration on the final results. Although for the very simplest model experiments analytic results have been obtained, realistic models of gamma-ray and neutron scintillation spectometers will require large-scale computer calculations, amounting to several hours' time on the IBM 7090.

A report on the results of this work [1] was presented at the Ninth Scintillation and Semiconductor Counter Symposium in February 1964. Future work will be concerned with the

optimization of the answer in the face of experimental uncertainties beyond those inherent in counting statistics. Preliminary calculations indicate that the dependence on spectrometer energy calibration can be made less sensitive at the expense of complicating the computer calculations, but that computing time on the 7090 may become prohibitive with this complication.

[1] Detenbeck, Robert W., Unscrambling pulse-height spectra on-line, Technical Report No. 362, Department of Physics and Astronomy, University of Maryland, 1964.

(11) Long Wave Length Radio Astronomy Research

Principal Investigator: Dr. Wm. C. Erickson, Associate Prof.
Physics and Astronomy

Since early summer 1963 the operation of the Clark Lake Radio Observatory in California has been taken over by the University of Maryland. Professor W. C. Erickson is directing the research work with this antenna.

The general purpose of this research work is to study phenomena at the long-wave length end of the radio spectrum with an antenna of very high angular resolution. This end of the spectrum is of great interest for many programs, and it is almost entirely unexplored. Thus far, studies in this wavelength range have been limited to the determination of the spectra of the 3 or 4 discrete radio sources (1), (2), observations of the decametric radiation from Jupiter (3), (4), solar observations (5), and a survey of the radiation from the southern portion of The Galaxy (6).

The interesting effects to be observed arise primarily from two causes. First, the spectra of discrete, non-thermal radio sources and the spectrum of The Galaxy rise with wavelength while those of thermal sources fall. Therefore, long wavelength observations yield data concerning non-thermal emission which are almost entirely free from contamination due to a thermal component, and are very useful for distinguishing between the different mechanisms of generation. This high intensity of non-thermal emission makes many types of observations feasible only at long wavelength. In addition, there is evidence that the halo radiation from radio galaxies grows increasingly intense relative to the central component as the wavelength increases. Secondly, many intriguing effects are caused by the fact that the opacity of ionized media and the departure of their indices of refraction from unity rise as the square of the wavelength. This permits the study of HII regions in absorption against the "hot" galactic background (6), very accurate studies of the refractive scattering of radio waves in the solar corona (7) and various ionospheric studies (8).

Following is a description of several observing programs which are now under way or are in the planning stages:

(1) Occultation observation -- Observations of the scattering of radio waves by coronal irregularities can yield data concerning electron densities in the corona, fluctuations in the density, and the coronal magnetic field distribution. During the summer of 1963, occultation observations of Tan A have been performed in order to study the morphology of the corona progressively throughout the solar cycle. Additional observations are to follow.

(2) Solar emission observations -- The declination coverage of the Clark Lake antenna is restricted, and sensitive observations can be made only north of the celestial equator. Therefore, solar observations are feasible only in the summer. The antenna has been engaged in such observations during the summer until September 1963. Since the sun and Tan A are at nearly the same declination during the occultation, occultation and solar emission studies can be performed simultaneously.

These observations have three goals. One will be the determination of the brightness distribution of the quiet sun at the 11.4 m wavelength of the antenna. This is expected to yield valuable data for insertion into models of the temperature and density distribution of the corona.

A second goal is the observation of more Type III emission events. These should give better determinations of the brightness distribution of these bursts, and plasma levels in the corona.

A third goal of the observations is the further study of Type I emission. Emission of this spectral type at our wavelength is frequently constant enough in amplitude that our drift scans may be expected to yield detailed information concerning the brightness distribution of the emission region, and to detect the presence of scattering halos if they exist for this emission.

(3) Discrete radio source studies -- Starting in the fall of 1963 the research effort has been concentrated on filling out the sky survey, and on obtaining high quality data concerning all regions of the sky from declinations 0^{o} to $+60^{o}$. It is expected that accurate observations of about 50 to 100 discrete sources can be obtained. It is hoped that these observations yield interesting data concerning source brightness distributions and halos; interesting

sources will be studied intensively with repeated fan beams scans, and with the roster of pencil beam scans.

All observational work under this research program depends of course crucially on the use of large scale computers for the data-reduction and analysis. In order to prepare for the future extensive computational work connected with this data-reduction and analysis a basic set of special and particularly efficient computer programs has already been prepared. In particular, two such basic programs are completely operational. The first program takes the raw data as it is produced by the telescope, makes all corrections for beam width, position, precision, and the like, and yields processed data concerning the position, angular size, and intensity of radio stars. The second program is used in the reduction of solar data. It solves various spherical trigonometrical problems. For each observation day it computes the position of the sun in each of the 70 lobes of the antenna's response pattern along with various other parameters such as the great circle distances between the sun and certain radio sources.

Other programs are being developed as the need arises, and it is obvious from the above general description of the research plans that the project will involve a growing heavy amount of computer use.

This work is now being supported under an NSF grant and is no longer receiving support under this contract.

References:

Flux Measurements of Cassiopeia A and Cygnus A between 18.5 MC and 107 MC, H. W. Wells, Proc. IRE, 46, 205, 1958.

The Radio Emission Spectrum of Cassiopeia A at Frequencies Below 30 Mc/s, S. Ya. Brande, A. V. Men, I. N. Zhuk, K. A. Babenkov, Astron. Zh., 39, 163, 1962 or Soviet Astron. --AJ, 6, 122, 1962.

Observation of a Variable Radio Source Associated with the Planet Jupiter, B. F. Burke, K. L. Franklin, J. Geoplup. Res., 60, 312, 1955.

Recent Decameter-Wave-Length Observations of Jupiter, Saturn, and Venus, T. D. Carr, A. G. Smith, H. Bollhagen, N. F. Six, Jr., N. E. Chatterton, Astrophys. J., j34, 1961.

The Extension of Solar Radio Spectroscopy to the Long-wave Limit Imposed by the Ionosphere, K. V. Sheridan, C. F. Attwood, Observatory 82, 1955, 1962.

A High Resolution Galactic Survey at 19.7 Mc/s, C. A. Shain, M. M. Komesaroff, C. S. Higgins, Aust. J. of Phys., 14, 508, 1961.

The Radio Wave Scattering Properties of the Solar Corona, (in press)
Ionospheric Refraction in Radio Astronomy. I. Theory, (together with M. J. Komesaroff), Aust. J. of Phys., 13, 153, 1960
Radio Emission in the Outer Corona, Phys. Rev. Letters 3, 365, 1959
Observations of 26.3 Mc/s Solar Radio Noise during August 1959, J. Geophys. Res. 66, 1773, 1961
High Resolution Studies of Type II Solar Emission at 11.4 m Wavelength, J. Geophys. Res., 68, 1963
The Occultation of the Crab Nebula by the Solar Corona in June 1959, P.A.S.P. 72, 167, 1960
Occultation of the Crab Nebula by the Solar Corona, June 1960, (together with P. Brissenden), P.A.S.P. 74, 1962

(12) Mass Transfer Between a Dispersed Liquid and a Liquid Continuum

Principal Investigators: Dr. R. B. Beckmann, Prof. and Head
Dr. A. Gomezplata, Assistant Prof.
Department of Chemical Engineering

All of the efforts to investigate the fundamentals of the mass transfer mechanism from dispersed liquid droplets have used a "model" approach. A fundamental model is devised which will permit a mathematical and computational approach to the interrelating factors of mass transfer, hydrodynamics, and interfacial phenomena.

The Basic Model: In a two-phase liquid-liquid system with a single transferring solute the mass transfer coefficient is most readily presented if the model configuration consists of one liquid phase dispersed in the other and in contact with it along a spherical surface. The two liquid phases are treated as continuous media and the interface is regarded as a mathematical surface subject to a normal stress (surface tension) and capable of supporting a two-dimensional stress tensor. Further, the two phases are assumed to be in mechanical equilibrium at the boundary.

The determination of the mass transfer for the model just outlined depends upon the ability to combine the effects of hydrodynamics, diffusional transport, and interfacial behavior on the passage of the solute between the two liquid phases. Generally, the viscosity, density, and surface tension of the liquid phase will depend upon the concentration of the transferring solute so that the differential equation describing the hydrodynamics, the diffusion, and the surface will be coupled.

However, if the solute is sufficiently dilute, the density and viscosity may be taken as constant and the flow and diffusion equation will be coupled only in the convective terms of the diffusion equation. In this case the flow equations are the standard Navier-Stokes equations and the continuity equation for incompressible, axially symmetric Newtonian flow. The concentration changes within an arbitrary two component phase as idealized in the model are governed by the equation

$$(1) \quad \frac{C}{t} + \text{div}(C\ V) = \text{div}\ (D + E)\ \text{grad}\ C$$

which relates the concentration to both time and position. The diffusion equation is obtained by applying this equation to a dispersed spherical element and to the continuous phase. The problem is completely specified by requiring that phase equilibrium exists at the interface and that the flux of solute across the interface be continuous.

Hadamard has shown that for a droplet in creeping flow (quadratic terms are neglected in the flow equations) a spherical shape is maintained with no oscillatory motions. Under this assumption the flow equations can be integrated and yield the well known Hadamard streamline equations. These Hadamard streamline equations may be combined with the general diffusion equation (1). Assuming that there is no resistance to transfer in the continuous phase, this yields:

$$\frac{\partial C_D}{\partial t} = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right)C_D + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right)C_D + \sigma(1-r^2)\cos\theta \frac{\partial C_D}{\partial r} + \frac{1}{r}(2r^2-1)\sin\theta \frac{\partial C_D}{\partial \theta} \tag{2}$$

where

$$\sigma = \frac{1}{3}\frac{g(\rho_d - \rho_c)}{3\mu_d + 2\mu_c}\frac{a^2}{D}, \quad C_D(a,\theta,t) = 0$$

Kronig and Brink have solved equation (1) for the limit $\sigma \to \infty$. Under the direction of R. B. Beckman and using the G-20 computer of the Carnegie Institute for Technology, L. E. Johns in 1960/61 successfully solved numerically the problem (1) for general values of σ.

R. Beckmann and A. Gomezplata are now extending this work to drop-side and continuous models in order to include a wider range of flow conditions as well as continuous phase and interfacial resistance. More precisely the objectives of this theoretical and exprimental research program can be summarized as follows:

(1) The development and generalization of a continuous, basic model for mass transfer between a dispersed liquid drop and an immiscible liquid continuum. The basic model is now being generalized to enable the numerical prediction of fundamental transfer rates on the basis of physical and thermodynamic data and transport information.

(2) An experimental program of mass transfer (liquid-liquid extraction) to and from single drops to aid in the development of the continuous, basic mass transfer model. Attention is primarily focused on non-aqueous systems and the

study of isothermal droplet transfer rates over a wide termperature range to gain the maximum variation in the governing physical and transport property parameters.

The computational problems arising in this research program are very formidable and are expected to demand a large amount of computer time.

(13) Turbulent Transport Coefficients

Principal Investigator: Dr. J. M. Marchello, Associate Prof.
Department of Chemical Engineering

Since Reynolds first suggested that heat and momentum are transferred by identical mechanisms, a number of investigators have proposed analogies between mass and heat transfer and momentum transfer in conduits. The problem is for the most part one of fluid mechanics, since it is necessary to describe the fluid behavior in detail in order to evaluate the mass and heat transfer characteristics. In particular, it is necessary to compute the profiles and transfer rates by integrating the flux equations, and, in turn, this integration can only be carried out if the dependency of the local flux and of the eddy coefficients upon position is known.

The turbulence present in the bulk of the fluid is suppressed in the vicinity of the solid surface. The early work with fluid mechanics and heat transfer assumed that a laminar sublayer existed at the surface. Recently several investigators (see e.g. (1)) have shown that this assumption of a laminar film at the solid surface leads to the erroneous conclusion that at low values of the diffusivity (high Prandtl or Schmidt numbers) the over-all transfer rate is proportional to the first power of the diffusivity. The major portion of the theoretical investigations of the eddy coefficients have been for isotropic turbulence. For non-isotropic turbulence, Corrsin has conducted a theoretical investigation of the eddy transport coefficients using Taylor's theory of diffusion by discontinuous movements. In a similar but somewhat more direct analysis, Jenkins (2), (3) used a modification of the Prandtl mixing length theory to predict the characteristics of the eddy coefficients. However, Jenkins himself already pointed out that his predictions of the eddy ratio cannot be expected to apply in the low levels of turbulence where the momentum eddy diffusivity and the kinematic viscosity are approximately equal.

Recently J. Marchello (4), (5) extended the basic principles of the penetration model in generality and applied the model to turbulent transfer data. From a comparison of the model predictions with the data, it can be concluded that the film-penetration model represents the fluid behavior in the low turbulence level which exists near the solid wall.

The penetration model results agree with Jenkins' conclusion that the eddy ratio may be represented as a function of the molecular Prandtl or Schmidt number and the momentum eddy diffusivity. However, the numerical values predicted by the two models differ considerably. When the momentum eddy diffusivity approaches zero, the fluid flow becomes laminar and the eddy diffusivities of heat and mass should also approach zero. The penetration model is consistent with this conclusion, but the Jenkins model is not. On the other hand, for the high turbulent Prandtl and Schmidt numbers should approach unity. The penetration model is not consistent with this conclusion, while the Jenkins model is. These observations indicate again that perhaps the Jenkins model applies in the turbulent core and the penetration model applies in the immediate vicinity of the wall.

J. Marchello and several of his graduate students are now investigating the variation of the eddy diffusivity of mass with molecular diffusivity. This research project consists of a coordinated experimental and theoretical investigation of the eddy transport coefficients with the following main objectives:

(1) To develop and employ the necessary computer programs for the computation of the concentration and temperature profiles and the mass and heat transfer coefficients.
(2) To examine the validity and range of applicability of current theories of turbulent transport.
(3) To determine experimentally the eddy diffusivity of mass and momentum in turbulent flow for a wide range of systems properties.

The computational work is in part based on the analogy techniques as used earlier by J. Marchello (6), as well as on a direct numerical integration of the fundamental equation of change of mass transfer in a fluid when applied to the case of a state injection from a point source. This equation has the form

$$\bar{u}\frac{\partial \bar{c}}{\partial x} = (\epsilon_D + D)\nabla^2 \bar{c} + \nabla \epsilon_D \cdot \nabla \bar{c}$$

where c is the concentration, u the axial velocity, D Fick's law diffusivity, ϵ_D the eddy diffusivity of mass, and the bar refers to time average values. As mentioned above, for the purpose of this research project, numerical solutions have to be developed for the case when ϵ_D and u varies with position.

For CO_2 in air at Re = 10^4 have been measured at various radial positions. Work on H_2 and u-octane is in progress. The computer program to calculate from the data has also been written and used for the CO_2 data.

REFERENCES

R. G. Deissler, Nat'l. Adv. Comm. Aero. (now NASA), TR 1210, 1955.

R. Jenkins, Ph.D. Thesis, Calif. Inst. of Technol. Pasadena, 1950.

R. Jenkins, Heat Transfer and Fluid Mechanic Institute Preprints, Stanford Univ., 147, 1951.

J. M. Marchello, H. L. Toor, Film Penetration Model for Man and Heat Transfer, A.I.Ch.E. Journal, 4, 97, 1958.

J. M. Marchello, Ph.D. Thesis, Carnegie Inst. of Technol., Pittsburgh, 1959.

J. M. Marchello, H. L. Toor, Ind. Eng. Chem. Fundamentals Quarterly 2, 8, 1963.

(14) Geophysical Fluid Dynamics

Principal Investigator: Dr. A. J. Faller, Research Associate Professor, Institute for Fluid Dynamics and Applied Mathematics

Dr. Faller and his assistants have begun a large-scale experimental and theoretical research study concerning rotating laboratory models which simulate atmospheric and oceanic circulations. This entire research work will depend crucially on the use of large-scale computers. More specifically there will be two types of computer use:

a) Data Reduction. One of the major problems of experimental fluid dynamics is the problem of tracing and analyzing the fluid motion. In Dr. Faller's experiments this will be accomplished by motion picture photography of discrete tracer elements; sometimes neutrally buoyant bubbles in the interior of the fluid, and sometimes floating tracers to indicate the free-surface circulation. The position of these tracers relative to a grid will be read from the films and entered on punch cards. It will then be necessary to apply corrections for parallax and refraction and for various other distortions. Later, the computed and corrected velocities will be used to compute various statistical measures of circulation, momentum and energy transport, and other properties of the flow.

b) Numerical Prediction Studies. An integral part of the research program will be the numerical prediction of fluid circulations in rotating tanks. These circulations will be in some cases similar to the general circulation of the atmosphere, and the uses and limitations of numerical prediction methods will be tested in these rotating fluid "models". In other studies the model experiments will simulate oceanic circulations or smaller scale phenomena.

Initial work in this direction has been reported by Mr. H. Sundquist (1963) who made numerical predictions of fluid circulations in a rotating tank under Professor Faller's supervision while in Stockholm.

In that study, a circulation was generated mechanically in a 1-meter square rotating tank with water 10 cm. deep. The observed circulation, which was recorded and measured by analyzing motion picture film of tracers on the free surface, was predicted using a finite-difference formulation of the approximate time-dependent hydrodynamical equations. In this

case the hydrodynamical equations were very much simplified to correspond to the laboratory system. Specifically, for slow motion in a rotating system and with a uniform fluid, the motion is independent of the rotating system and with a uniform fluid, the motion is independent of the vertical direction (along the axis of rotation), and the viscous boundary layer at the bottom of the fluid may be "paramaterized" in a rather simple fashion. Under these circumstances the problem becomes two-dimensional, although non-linear and time dependent, but the approximate equations are an excellent representation of the state of motion of the fluid, and measurements of the free surface flow completely describe the motion.

Such conditions are seldom satisfied in the atmosphere where the fluid is compressible and stratified, the motion has important variation with height and is basically three dimensional, and the observational coverage is generally inadequate. Under such circumstances it is difficult to separate the various sources of error in prediction which may arise from (1) inadequate obervations, (2) faulty numerical techniques, or (3) poor representation of the true flow field by the approximate hydrodynamical model.

Thus the use of models provides a systematic method of assessing the relative importance of these sources of error in a system which is in many respects similar to its prototype. The experimental model and the corresponding numerical model may be complicated in successive stages gradually to approach the prototype situation.

As a specific example of the type of equation to be solved, I cite equation (4) of Sundquist (1963) which was derived with some of the simplifying assumptions stated above. This equation for the stream function of the flow is:

$$\frac{\partial \nabla^2 \psi}{\partial t} = - J(\psi, \nabla^2 \psi) + D \nabla^2 \psi$$

where ψ is the stream function, $\nabla^2 \psi = S$ is the vorticity of the two-dimensional flow, J is the Jacobian and D is a frictional coefficient. The initial application was to the determination of the initial field of stream function from velocities observed at fixed grid points on a 20 x 20 grid. The velocities were first used to find the voriticity S, and with appropriate boundary conditions the field of ψ was determined by relaxation. The above equation was then iterated to obtain predicted values of ψ at later times for comparison with observed circulations.

The above procedure may be described as the Eulerian prediction method, since the changes of a quantity at fixed spatial points are to be found. While this method gave rather accurate results for one case for four revolutions of the tank (4 days), it should be extended to experiments with different values of the circulation parameters and it should be compared with other prediction methods. Other systems which have been advanced for use in meteorological forecasting are the Lagrangian advection method proposed by Fjortoft (1952) and the use of Fourier analysis, where the changes of the Fourier coefficients which described the field of ψ would be predicted. Furthermore, it is not necessary and may be unwarranted to describe the motion in terms of a stream function. An alternative is the use of the so-called "primitive" equations where the velocity of vorticity field is directly predicted.

Thus even with this very much simplified experimental model, there are many corresponding numerical models for the description of the change of circulation. The sources of error should be isolated and clearly determined for the various numerical methods so that their relative advantages and deficiencies are clearly understood. Only when this understanding has been achieved may the experimental and theoretical models be advanced to the next stage of complexity.

Our ability to predict laboratory circulations with a given prediction technique will indicate an upper bound to the predictability of atmospheric and other planetary circulations using that same technique. This conclusion, of course, rests upon the assumption that the dominant dynamical processes which occur in the model are the same as in the prototype, and that the same degree of observational coverage and accuracy or better may be attained.

The above description is intended to describe only the philosophy behind the research project and the general procedure to be employed. The case presented here is the simplest possible example and generally the prediction equations to be iterated will become more sophisticated as re-

Methods of numerical prediction similar to those described above have recently been employed by Dr. Faller and Mr. Kaylor in the study of the stability of rotating boundary-layer flows analogous to the turbulent boundary layer in the atmosphere.

These numerical experiments have their origin in laboratory experimental results where instability of the Ekman boundary layer was observed and where some characteristics of this instability were determined (Faller, 1963). By means of numerical iteration of the time dependent equations of motion it has been possible to determine the form of the unstable perturbations for Reynolds numbers above the critical value and to determine the rate of growth of amplitude of these perturbations. These results are in excellent agreement with the experimental findings and the numerical technique shows great promise. The laboratory results may be extended far beyond those results that readily may be determined by laboratory experiment.

The numerical experiments will be continued and expanded in order to determine:

a) The growth rates of unstable perturbations and their equilibrium finite amplitudes as a function of Reynolds number and other paramters.

b) The shape of the curve of critical Reynolds number vs. wave number for neutral stability.

c) Stability criteria and other characteristics of the instability for boundary conditions relevant to the surface layer of the oceans, and

d) Stability criteria, growth rates, and equilibrium amplitudes for turbulent boundary layer flows corresponding to natural situations.

References:

H. Sundquist, A numerical forecast of fluid motion in rotating tank and a study of how finite-difference approximations affect non-linear interactions. Tellus, XV, 44-58, 1963.

R. Fjortoft, On a numerical method of integrating the barotropic vorticity equation. Tellus, IV, 179-194, 1952.

P. D. Thompson, Numerical Weather Analysis and Prediction. The Macmillan Co., New York, 170 pp., 1961.

A. J. Faller, An experimental study of the instability of the laminar Ekman boundary layer. J. of Fluid Mechanics, 15, 560-576, 1953.

A. A. Townsend, The Structure of Turbulent Shear Flow, Cambridge Univ. Press, 315 pp., 1956.

(15) Abstracts of selected additional computer oriented research projects

This section presents a selection of a number of additional space related research projects in the University which are strongly computer oriented yet probably do not involve as extensive amounts of computer usage as the projects described earlier.

(a) The Conductance of 2-2 Salts in Water and Mixed Solvents

Dr. G. Atkinson, Assistant Professor of Chemistry

The purpose of this project is an investigation of the conductance of 2-2 salts in water and mixed solvents with the aim of beginning an analysis of the status of electrolyte conductance theory. Very recently Fuoss and Onsager reexamined some of the mathematical approximations underlying the 1957-59 version of the Fuoss-Onsager theory and proposed a new version that is mathematically more self-consistent. The form of the new equation is considerably more complicated than the original Fuoss-Onsager equation, and some preliminary numerical analysis shows that this new equation exhibits a rather strange behavior. It is now planned to take some of the best data on 1-1 and 2-2 electrolytes both associated and unassociated and fit it to the F-O-1957 and the F-O-1963 theories.

For a more complete analysis of the electrolyte conductance theories it is then planned to extend the analysis to the theories of Pitts and Kelby. Because of their very involved functional form, these theories have not been adequately analyzed numerically. All four theories give Λ, the equivalent conductance, as a function of three parameters: Λ°, the equivalent conductance at infinite dilution, a, the mean distance of closest approach, and c, the concentration. The theories are, therfore, directly comparable. By carefully choosing a variety of systems of widely differing conductance characteristics, this computer program should give results which provide a very good idea of the present status of electrolyte conductance theory.

Programming has been completed on three forms of the Fuoss-Onsager theory and extensive data analysis is being carried out.

(b) Theoretical Plasma Research

Dr. D. A. Tidman, Research Associate Professor, Institute for Fluid Dynamics and Applied Mathematics

Much (and probably most) of the basic theory required to understand the complex plasma phenomena occurring in the Solar System is not yet developed. To mention only one example: Type II solar radio outbursts are thought to originate in shock fronts in the solar corona but there is no plausible theory of plasma shock waves as yet. Under Dr. Tidman as principal investigator a group of plasma physicists are directing their research into the fundamental kinetic theory of plasmas based on the approach of the B-B-G-K-Y hierarchy of equations and parallel with attempts to understand space plasmas.

Most parts of this research work lead ultimately to problems of numerical computations. A typical one of these problems is presently nearing completion: The one particle distribution function, f, for an electron plasma obeys the Balescu-Lenard equation. [$f(\underline{x},\underline{v},t)\,d\underline{x}\,d\underline{v}$ = probable number of electrons in the velocity element $d\underline{v}$ and space element $d\underline{x}$ at time t]. This equation describes how f changes due to Coulomb collisions between electrons.

In the first part of the investigation the relaxation to equilibrium was computed for a number of isotropic distributions. [The Balescu-Lenard equation simplifies considerably for homogeneous plasmas in which the electron velocities are isotropic, i.e., $f(\underline{x},\underline{v},t) \rightarrow f(|\underline{v}|,t)$]. Mr. A. Dolinsky has computed the characteristic times in which fine structure in velocity space is wiped out due to Coulomb collisions. The results have been compared with the corresponding results from the Fokker-Planck kinetic equation of Rosenbluth, MacDonald, and Judd.

This entire line of computational work will be continued with other kinetic equations

(c) Model Atmosphere for Cepheid Variables

Dr. R. Bell, Assistant Professor of Physics and Astronomy

Dr. Bell's present research interests are in the field of Cepheid variable stars. He has been taking spectra of

these variables with the 74-inch reflector at Mount Stromlo, investigating the pressure and temperature changes during the pulsation. The analysis of the dispersion spectra of these stars involves a considerable amount of computer work. Various programs have been written or are now in the planning stages. A first program computes the line profiles for a Milne-Eddington atmosphere. Another program is designed to compute hydrogen line profiles and continuous spectral energy distributions for model stellar atmospheres. Model atmospheres are obtained as the solution of certain ordinary differential equations for the pressure P and the temperature T as functions of optical depth τ. The continuous spectrum is then computed from the model atmosphere by evaluating the optical depth at different frequencies and then calculating the integral for the flux. The hydrogen line profiles may be obtained by computing the variation of the absorption coefficient away from the line center and evaluating the flux emitted by the star at wavelength up to about 10 A^{o} from the line center.

As a next phase of the project, it is planned to calculate flux constant models in which $F = \int_0^\infty F_\nu(\tau) d\tau$ is constant with optical depth.

Another project which is being investigated in cooperation with Dr. A. W. Rodgers is the following:

It appears, from current work on cepheid variable stars and supergiant stars, that the macroturbulent velocity is a function of the strength of a line and presumably a function of the height in the stellar atmosphere at which it is formed. This result has been obtained using only simple representations of stellar atmospheres but appears to be confirmed by solar observations. It is hoped to investigate the matter further using more complex broadening functions and more elaborate stellar atmospheres. This further investigation will need to be performed numerically. The problem is presumably related to the H and K reversals found by O. C. Wilson.

(d) Nuclear Reactions and Optical Potential

Dr. W. MacDonald, Professor
Dr. A. Altman, Assistant Professor
Department of Physics and Astronomy

The investigators have recently developed a unified theory of nucleon reactions which makes possible a phenomeological analysis including both direct and resonant amplitudes. Application of the theory will now be made to analyses of (n,p), (p,n), (d,p), and (d,n) reactions using the IBM 7090. In addition, it is planned to extend the theory to the treatment of reactions involving deuterons and more complex particles.

Previous computations of the optical potential have been limited mostly to the case of high energy nucleons on nuclei. The approach of the above unified theory appears to make feasible computations of the nucleon optical potential for low energy reactions on light nuclei. In addition, the problem of extending the theory to derive the optical potential for deuteron reactions will be considered in the same frame-

(e) Effect of Configuration Mixing in the Universal Fermi Interaction

Dr. W. MacDonald, Professor
Dr. A. Altman, Assistant Professor
Department of Physics and Astronomy

The conserved vector current theory of the universal Fermi interaction predicts equality of the polar vector coupling constant G_V for β decay and the coupling constant G_μ for μ decay. The most accurate determination of G_V is from the measurement of the ft value for the $0^+ \rightarrow 0^+$ decay of O^{14} to the first excited state of N^{14}. The value G_V^2 obtained is found to be smaller than G_μ^2 by approximately 2%. The decrease in the nuclear matrix element produced by the Coulomb interaction was computed by MacDonald using jj-coupling and antisymmetrized wave functions and considering configuration mixing arising from excitation of a 1p nucleon to a 2p state and found to be an order of magnitude too samll to explain the discrepancy. The charge dependent nuclear force suggested by Blin-Stoyle and Le Tourneax and determined for the A = 14 system by Altman and MacDonald was considerably too small to give the required reduction of the nuclear matrix element. Suggestions that configuration mixing and excited collective states may contribute to the decrease in the matrix element have been made but never computed. Such computations are now planned.

(f) Analysis of a Helium-Scattering Proton Polarimeter

Dr. R. Detenbeck, Assistant Professor of Physics and Astronomy

Distorted-wave theories of (d,p) reactions have recently given greater insight into the mechanisms of these reactions

and promise to make them even more powerful experimental tools for the study of nuclear structure in the future. One of the most critical tests for any distorted-wave reaction theory is the prediction of the polarization of the outgoing particles.

The University of Maryland Van de Graaff accelerator has been used to study the polarization of protons from the $He^3(d,p)He^4$ reaction for deuteron energies between 2 and 3 MeV. The polarization was measured as an asymmetry in the scattering of the emergent protons to right and left from helium gas. In order to deduce the polarization p_1 of the scattered protons from the measured asymmetry A, it is necessary to know the effective analyzing power P_{eff} of the helium polarimeter ($A = P_1 \quad P_{eff}$).

The effective analyzing power of the polarimeter can be calculated from a knowledge of the polarimeter geometry and the p-He^4 scattering phase shifts. Even for point geometry the computational work is complex and very demanding on computer time. In particular, for the $He^3(d,p)He^4$ experiment the outgoing protons vary in energy from 12 to 20 MeV and a very detailed computer analysis has to be undertaken to make use of the known smooth energy dependence of the p-He^4 (second scattering) phase shifts which permit polarization analysis over such a wide energy range.

The analysis is now nearly complete and the results are being written into Mr. Huoo Long Fann's Ph. D. dissertation and also will be prepared for publication. A short talk at the New York American Physical Society meeting, January 1964 has been given on the preliminary results of the experiment.

(g) Giant Dipole Resonance -- Collective Level Shift Computations

Dr. W. Greiner, Assistant Professor of Physics and Astronomy

The shell-model theory of the giant dipole resonance is based upon starting with accurate single-nucleon wave functions as solutions of the Hartree-Fock self-consistent field. When only bound state wave functions are involved, reasonable accuracy can be obtained by the harmonic oscillator approximation. This is, however, no longer true in

the more realistic situation where the important excitations are free, or unbound states of the nucleus. In this case the single-nucleon wave functions are in reality scattering states and lend themselves to no simple analytic approximation. It is necessary to evaluate them numerically on a computer.

This project is presently concerned with investigating the shift of the collective giant-resonance levels in O^{16} due to the interaction of these bound levels with continuum states. This interaction takes place via residual forces, which have not been included in the shell-model field.

The computations undertaken so far have shown that the neutron emission is of the order of 0.6 MeV, a quite appreciable correction to the usual particle-hole calculations.

The work is now continuing with the computation of the same effect for virtual proton emission. For this purpose it is necessary to develop special programs for the evaluation of regular and irregular Coulomb wave functions.

(h) Diffusion Mechanism for Ion Exchange

Dr. J. M. Marchello, Asst. Prof. of Chemical Engineering

The project is concerned with the rate of ion exchange for thin packed beds and for agitated or stirred beds. The mechanism of ion exchange and the rate determining steps are fairly well understood from a qualitive standpoint. However, the prediction of exchange rates has not yet been satisfactorily treated.

Dr. Marchello together with one of his doctoral candidates, J. P. Copeland, has developed the equations which describe the diffusion mechanism and which can be used to obtain the surface flux. The theoretical development is based on the differential equations of the material balance and the component balance. The new relations have already been used to investigate the absorption of dilute complex-thorium nitrate from concentrated HNO_3 with Dowex 1-X4 resin.

It is now planned to use the new method to reexamine existing theories and models of ion-exchange kinetics.

(16) Projects Presently Completed Or Nearing Completion

For the sake of completeness we here present brief descriptions of those research projects which were supported under the grant during the first year and which now are either completed or which will be completed within the next few months. Among those projects nearing completion, only those have been included here for which no continuation is currently anticipated.

(a) Computer Applications to Group Theory

Dr. A. Sinkov, Computer Science Center*
J. W. Snively, Jr., NASA-Trainee, Computer Science Center

In the last few decades, group-theoretic problems have gained increasing importance in a number of applications, ranging from quantum-mechanics to cryptography. But only in recent years has attention been directed toward the use of computers in group-theoretic research.

A basic problem in the theory of groups is the determination of the group defined by a set of relations satisfied by its generators. The coset enumeration technique of Todd and Coxeter (Proc. Edinburgh Math. Soc. (2), 5, 1936) is sufficiently mechanical to admit of being programmed for a high speed computer. Several investigators have worked at the problem of programming it. Most of this work is as yet unpublished. A first paper concerning this topic was published by J. Felsch, (Num. Math. 3, 250, 1961); he used a Zuse Z-22 computer. Recently a paper by J. Leech (Proc. Cambridge Phil. Soc. 59, 257, 1963) described his work on the EDSAC-computer. During the past half year the investigators developed IBM-7090 programs for this enumeration process.

A comparison of these three programs is available for the case of a test problem; namely, for the enumeration of a group defined earlier by A. Sinkov (Annals of Math. 38, 3, 1937). A pencil and paper enumeration by Todd required in excess of 30 hours, Felsch used 2 hours on the Z-22, Leech used 42 minutes on the EDSAC and Sinkov used 5 minutes on the IBM-7090.

---

* Now: Department of Mathematics, Arizona State University, Tempe, Arizona

This enumeration procedure is being used to study the Burnside problem of exponent 4, about which very little is known. $B_{4,1}$ is trivial and of order 4; $B_{4,2}$ is of order 2^{12}. The only other known result is that $B_{4,n}$ is finite.

The IBM-7090 programs for the computer enumeration have produced the following results to date:

1. An irreducible definition of the 2-generator methabelian group of exponent 4.
2. The order of $B_{4,3}^{(3)}$ (where the superscript means that 3 generators are involutary) is 2^{10}.
3. The order of $B_{4,3}^{(2)}$ is 2^{21}.
4. A procedure has been indicated by which the orders of $B_{4,n}^{(\alpha)}$ may be derivable from the establishment of a chain of invariant operators and corresponding quotient groups. These invariant operators -- for all cases tried thus far -- are commutators or squares of commutators.
5. This procedure -- if effected -- will simultaneously provide a definition of a Brunside group of exponent 4 for every power of 2 starting from that which gives the order of $B_{4,n}^{(\alpha)}$ down to $2n-\alpha$.
6. It is indicated that the extension from $B_{4,n}^{(\alpha)}$ to $B_{4,n}^{(\alpha+1)}$ causes the exponent of 2 to be at least doubled.

Dr. Sinkov's results have been reported to NASA in our Technical Note (1) dated September 1963.

Under Dr. Sinkov's direction, James Snively, Jr. used the enumeration logic developed by H. Felsch's (loc. cit.) further computer work on the same problem. In particular, J. Snively succeeded in finding a definition for the Burnside group $B_{3,4}$ of exponent 3 with 4 generators which involves only 35 words. J. Snively just completed a Technical Report (2) describing his work as well as summarizing the work of others on digital computer programs for the automatic enumeration of cosets. This report has been submitted to NASA

(1) A. Sinkov, A Computer Application to Group Theory
Computer Science Center, Univ. of Maryland
Technical Note TN-63-1, September 1963

(2) J. W. Snively, Jr., The Use of Digital Computers to Determine Definitions for Abstract Groups
Computer Science Center, Univ. of Maryland
Technical Report TR-63-4, November 1963

(b) Numerical Analysis in Modular Arithmetic Computers

G. E. Lindamood, Research Programmer, Computer Science Center

Modular arithmetic computers--digital computers in which numbers are represented by their residues with respect to several mutually prime moduli--have recently been the subject of considerable investigation in several universities and private companies in the United States and in the Laboratory of Mathematical Machines in Prague, Czechoslovakia. Of particular interest in these investigations have been the theoretical problems arising in performing several fundamental operations, such as overflow detection, magnitude comparison, and division in these computers.

As a result of work beginning in June 1962, at Westinghouse Electric Corporation in Baltimore, Maryland, G. E. Lindamood has found mathematical techniques for comparing the magnitudes of two numbers, detecting additive and multiplicative overflow, performing division, and extracting square roots in modular arithmetic computers. These techniques are of the utmost importance in the development of modular arithmetic computers, since it was previously unknown how to perform these operations in the number system used in such computers. To demonstrate the practical application of these techniques, G. Lindamood prepared programs to simulate modular arithmetic division and square root extraction on the IBM 7090 computer. These programs have provided additional information about the speeds of convergence and general behavior of the modular arithmetic division and square root techniques.

G. Lindamood is currently preparing a report summarizing his contributions on performing the fundamental operations in modular arithmetic computers and presenting the results of the simulation runs.

Pertinent References

G. Lindamood & G. Shapiro: "Magnitude Comparison and Overflow Detection in Modular Arithmetic Computers" SIAM Review, Vol. 5, No. 4, pp. 342-350, October 1963.

(c) Chebyshev Approximations for Elementary and Special Functions

C. K. Mesztenyi, Senior Research Programmer, Computer Science Center
Dr. C. Witzgall, National Bureau of Standards

In all computational work elementary and special functions need to be evaluated repeatedly and efficiently. This has led in past years to an extensive development of approximations for these functions. One large-scale research project on the use of rational approximations for the uniform (Chebyshev) approximation of functions was carried out by H. Maehly at Princeton University and later on at Syracuse University. Dr. Maehly's death in 1961 interrupted this work after only a small part of the research results had been completely checked out and published. His direct collaborators, C. Witzgall (now with the Applied Mathematics Division of the National Bureau of Standards) and C. K. Mesztenyi (Senior Research Programmer at the Computer Science Center) are now collecting these earlier results in order to put them in final form for publication and then to continue this important research work.

Up to date, the following functions were approximated and checked out:

ARCSIN(X)
ARCTAN(X)
T(X)
log T(X)

with approximately 80 approximations for each. Partly finished functions are the following:

SIN(X)
COS(X)
TAN(X)
ERF(X)

Additionally approximations have been obtained for other functions (SQRT(X), EXP(X), LOG(X), BESSEL FET etc.), but as yet they have not been checked out.

(17) Abstracts of selected additional projects started since December, 1963

(a) The Interaction of Independent Variables and the Multiple Correlation Coefficient

James F. Williams, Computer Program Documentation Specialist, Computer Science Center.

In the prediction of future events, multiple regression is most frequently used. The assumption underlying this technique is that the dependent variable (criterion) is linearly related to each independent variable (predictor) and that this relationship is constant for different levels of the other independent variables. This assumption may be violated in two ways: (1) If there exists a curvilinear relationship between the dependent variable and one or more of the independent variables which remains constant for different levels of the other independent variables, and (2) if there exists a joint relationship, that is, if the relationship between the dependent variable and an independent variable changes for different levels of the other independent variables. In the latter case, a more complex regression surface would be needed to appropriately fit (least squares) the form of data.

Unfortunately, in most prediction situations, the standard multiple regression technique is used without determining the true form of variable relationships or allowing for the possibility of a joint relationship. The main reason for this being that the computations required are extremely laborious. Work, however, may be reduced to a minimum by utilizing digital computing techniques. It is the purpose of this study, through the use of the IBM 7090/1401 system at the Computer Science Center of the University of Maryland, to investigate the prediction of future events by making use of the more complex joint regression methods.

(b) Maximum Pressure Cold Stellar Models

C. W. Misner, Associate Professor, Department of Physics and Astronomy

The computations will construct equilibrium, zero temperature, spherically symmetric model of dense stars assuming an equation of state which supplies the maximum conceivable pressure (sound velocity equals light velocity) to resist colapse. It is anticipated that no such solutions

will exist above some critical mass. The computations solve two simultaneous ordinary differential equations and plot several quantities as function of the radius.

(c) Quantum Electrodynamics

H. C. Lam, Research Associate, Department of Physics and Astronomy

The electron propagator and the vertex function in quantum electrodynamics are investigated by a non-perturbative method in which linear and non-linear volterra type integral equations have to be solved. It is hoped that through the combined use of analytical and numerical methods that the solutions of these equations may be found. If a complete solution can be found, such questions as whether muon and electron can appear together in the present theory, and whether the photon can acquire a mass for strong enough couplings may be answered.

Non-linear volterra integral equations and differential equations will be solved to obtain the behavior of the electron propagator and the vertex function for various values of the coupling constant.

(d) Altitude and Mapping Program, Association for Lunar and Planetary Observers

L. E. Bragg, Research Assistant Professor, Institute for Fluid Dynamics

This project involves calculation of altitudes of lunar features using data supplied from time to time by amateur observers. The Omnitab Language will be used to compute feature height H, solar altitude A, and coordinates B and L from

$$\text{SINB} = \eta, \quad \text{SINL} = \mathcal{E}/\text{COSB}$$

$$\text{SINA} = \mu\,\text{SINB}'' + (\text{COSC} + [1-\epsilon^3\rho^2]^{1/2}\text{SINC})\text{COSB}''$$

$$\text{COSF} = \text{SINB}'\text{SINB}'' + (\text{COSB}'\text{SIN}(\text{L}'+\text{C}))\text{COSB}''$$

$$\text{H} = \left[\left(\frac{\ell}{R}\right)\text{SCSFSINA}\left(2 + \left(\frac{\ell}{R}\right)\text{CSCFSINA}\right) - \left(\left(\frac{\ell}{\rho}\text{CSCF}\right)^2\right]\right.$$

wherein all other variables except F are data. About fifty data points per three months have in the past been made available computations.

The project is coordinated by the Association of Lunar and Planetary Observers, and is performed on a volunteer basis by its members. The association publishes a journal, The Strolling Astronomer, on a non-profit basis, and coordinates the work of its amateur members. The project has been going on for about one year using desk calculators on small collections of data. It is expected to continue for two or three years, provided that data becomes available.

(e) Nuclear Reactor Codes

D. Duffey, Professor and Nuclear Reactor Director
Department of Chemical Engineering

The following is information on some of the computer codes to be tried; these codes pertain mostly to reactor physics analysis and related studies concerning nuclear reactor operations. Much of this is based on the Argonne National Laboratory Computer Library work.

1) Muft-5 - This program will solve the Pl or Bl multigroup neutron equation for the first two Legendre coefficients of the directional neutron flux -- flux and current-- and the isotropic and anisotropic components of the slowing down densities due to a cosine-shape neutron source. Hydrogen may be treated exactly or in a Selengut-Goertzel approximation. For energy degradation by heavy elements both age and Grueling-Goertzel approximations are available. Slowing down of neutrons by capture and fission resonances is included. Only the non-thermal energy range is considered.

2) Wanda-5 - This is a numerical solution of the one-dimensional few-group neutron diffusion equations. One to eight energy groups may be used and rectangular, cylindrical, or spherical geometry formulations are available. The flux or its derivative may be set to zero at the boundaries. The program will vary buckling or neutron poison cross section in any subset of regions, or the position of one or more interfaces separating regions to find a specified critical eigenvalue. One iteration or fixed source problems may be calculated and adjoint solutions may be obtained. All one-group problems are treated as one iteration problem.

3) Gam-1 - This program computes the slowing down spectrum in either the P1 or the B1 approximation using 68 groups of neutrons with a constant group width DU-0.25. The code calculates multigroup constants for up to 32 fast groups.

4) Tempest-11 - Tempest-11 is a neutron thermalization code based upon the Wigmer-Wilkins approximation for heavy moderators. A Maxwellian distribution may also be used. The model used may be selected as a function of energy. The second-order differential equations are integrated directly rather than transformed to the Riccati equation. The code provides microscopic and macrosxopic cross-section averages over the thermal neutron spectrum.

5) PDQ - This is a two dimensional multi-group, multi-region diffusion code.

6) There will be other codes particularly on the lines of the 3 dimensional codes, burn-out and reactivity codes, spectrum codes and disadvantage factor codes for nuclear reactors. Other codes related to nuclear reactor operations will be tried, e.g., data from the gamma ray multichannel analyzer will be fed to a code to identify kinds of and amounts of nuclides activated in neutron activation analysis work. There will be codes bearing on neutron and gamma ray shielding, heat transfer and stress analysis. The Monte Carlo Technique may be applied to neutron and gamma ray problems.

All these codes will be compatible with the IBM 7090 and programmed in FORTRAN language.

(f) Studies in Two-Phase Downflow Period

H. Pollack, Graduate Student, Chemical Engineering

The research under discussion is concerned with the study of phase distribution in the vertical flow of gas-liquid mixtures in both the upward and downward direction. Little work has been directed toward two-phase downflow and no correlation concerning the variation in phase distribution between upflow and downflow under variable conditions such as velocity, bubble size, and column diameter exists.

Collimated gamma beams will traverse the column and a series of average spatial densities will be obtained by use of a scintillation detector.

Assuming that the density can be expressed as a function of a third-order polynomial, the computer will be employed to calculate the coefficients of the polynomial by the method of least mean squares. Once the coefficients are known, the polynomial may be employed to obtain point densities which are a measure of the phase distribution. In addition, computer programming will be used to obtain the standard deviation of the measured density from that predicted by the polynomial.

(g) Numerical Solution of Systems of Non-linear Equations

J. M. Ortega, Research Assistant Professor
Computer Science Center

To obtain a numerical solution of n equations in n unknowns, the Newton-Raphson method is commonly employed. However, this method requires the use of partial derivatives which may be difficult or impossible to obtain. It is planned to investigate a class of similar methods which, however, require no derivatives. The investigation will be mainly theoretical but will also use the computer to test the efficacy of these methods in practice.

Numerical Solution of "Stiff" Ordinary Differential Equations

Certain differential equations are termed "stiff" if their solution contains short lived transients. The usual numerical methods, e.g. Runge-Kutta, for numerically solving differential equations are unsuitable here because of the very small integration step required. It is planned to investigate certain other methods which show promise of producing good approximate solutions for these equations with a reasonable amount of computer time.

Appendix I: List of Technical Reports

1. A Computer Application to Group Theory
   by A. Sinkov
   Techn. Note TN-63-1, Computer Science Center, Sept., 1963

2. On Sieves and Primes
   by S. Kuroda and J. Maryak
   Techn. Report TR-63-2, Computer Science Center, Oct., 1963

3. Multiple Precision Package, UOM-MPP, for the IBM-7090/7094
   by A. Beam
   Techn. Report TR-63-3, Computer Science Center, Oct., 1963

4. The Use of Digital Computers to Determine Definitions for Abstract Groups
   by J. W. Snively, Jr.
   Techn. Report TR-63-4, Computer Science Center, Nov., 1963

5. Macro Output Input System (MOIST) for the IBM 7090/7094
   by G. Berns
   Techn, Report TR-64-5, Computer Science Center, Jan., 1964

6. X-Ray-63, Crystallographic Computing System
   by J. Stewart
   Techn. Report TR-64-6, Computer Science Center, May, 1964

7. Numerical Analysis in Residue Number Systems
   by G. Lindamood
   Techn. Report TR-64-7, Computer Science Center, May, 1964

Appendix II: Table 1

COMPUTER TIME SUMMARY

April 1963 - March 1964

	Apr	May	June	July	Aug	Sept	Oct	Nov	Dec	Jan	Feb	Mar	Total
RECORDED TIME*													
I. Academic Use													
(Execution time only)													
College of Arts & Sciences	79	73	46	56	94	65	102	97	95	109	190	156	1162
College of Engineering	1	4	1	2	5	2	11	7	18	11	10	23	95
College of Business & Public Administration		1	15	28	15	3	5	3	16	11	6	9	112
College of Agriculture**	2	3	9	4	7	3	3	6	2	3	11	9	62
College of Education					1	2	2	1	1	3	5	1	16
School of Medicine	1	2	2	3	1	4	1	3	2	2	2	1	24
Computer Science Center	71	56	64	53	44	68	60	55	44	44	40	66	665
Cooperative Research with other Educational Institutions				8	10	6	10	1	1	11	14	1	62
Home Economics										1	1	1	3
Physical Education											1	1	2
Other Independent Units of the University										1	1	1	3
II. Computer Maintenance	36	22	24	29	46	33	33	38	23	33	26	69	412
III. Set-up Time***	87	79	77	84	91	83	89	81	71	79	80	78	979
TOTAL	277	240	238	267	314	269	316	292	273	308	387	416	3597
IV. Other Time (Including idle and unreported)	44	93	111	160	121	87	97	69	49	111	70	59	1071
CONSOLE LOG ON-TIME	321	333	349	427	435	356	413	361	322	419	457	475	4668

*Rounded to next full hour

**Includes Natural Resources Institute

***Time consumed before and after runs involving the executive-and sub-systems in control, the appropriate monitors, and required operator activity.

APPENDIX II Table 2

Table of Computer Time Supported by NASA Grant NsG 398

(All times are given in hours, minutes, and seconds)

	Prev.Tot.	Sept.	Oct.	Nov.	Dec.	Jan.	Feb.	Total
Programming Systems	61-10-08	14-1-41	16-1-44	27-53-5	14-50-9	26-50-25	18-31-53	179-19-5
Numerical Mathematics	69-28-12	3-59-59	6-41-36	0-44-14	5-3-49	2-5-22	3-14-14	91-17-26
Chemistry	69-43-26	9-54-49	6-53-43	16-46-5	2-56-17	13-48-53	65-12-28	185-15-41
Molecular Physics	1-22-22	0-7-5	0-37-41	5-50-15	5-57-54	8-9-3	12-54-1	34-58-21
Physics & Astronomy	14-31-11	2-39-3	6-51-39	8-25-17	13-26-18	14-7-17	7-2-45	67-3-31
Engineering	2-20-37	0-10-4	0-53-53	0-8-17	1-32-9	1-29-32	5-17-16	11-51-48
Pattern Recognition and Associated Statistical Investigations	--	0-12-37	0-15-13	1-9-39	1-6-47	3-17-13	2-37-35	8-39-4
Totals	218-35-56	31-5-18	38-15-29	60-56-52	44-53-23	69-47-45	114-50-12	578-24-56